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Band-structure effects in the spin relaxation of conduction electrons (invited)

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Spin relaxation of conduction electrons in metals is significantly influenced by the Fermi surface topology. Electrons near Brillouin zone boundaries, special symmetry points, or accidental degeneracy lines have spin flip rates much higher than an average electron. A realistic calculation and analytical estimates show that these regions dominate the spin relaxation, explaining why polyvalent metals have much higher spin relaxation rates (up to three orders of magnitude) than similar monovalent metals. This suggests that spin relaxation in metals can be tailored by band-structure modifications like doping, alloying, reducing the dimensionality, etc. © *1999 American Institute of Physics*. [S0021-8979(99)64908-8]

The ability of normal metals to carry a spin-polarized current has led to the development of spin transistor,[1] a ferromagnet-normal metal-ferromagnet sandwich device that can switch current depending on the relative orientation of the magnets. Spin polarized currents also flow in the metallic layers of giant magnetoresistance heterostructures,[2] substances promising for magnetic signal processing. A major limitation of the quality of these devices is imposed by the time (the so called spin relaxation time T_1)[3] an unbalanced spin population in metals persists; the metallic layers used in these devices cannot be thicker than the spin diffusion length which is proportional to $\sqrt{T_1}$. Finding ways of enhancing T_1 is technologically important also from the perspective of quantum computing that represents bits by electronic spins.[4] One recent successful attempt to increase T_1 in semiconductors by doping is described in Ref. 5.

We recently reported[6] on a theoretical study of the spin relaxation in polyvalent metals where we showed how the band structure affects T_1. The physical picture is the one of a random walk on the Fermi surface: the weakness of the spin-flipping interactions in a typical metal ensures that an electron changes its momentum many times (typically a 10 000) before its spin flips. At some points (we call them *spin hot spots*), however, the spin-flip probability is much enhanced. Near a Brillouin zone boundary (Bragg plane), for example, this probability can increase a hundred times. If the electron jumps in or out of a special symmetry or accidental degeneracy point, the probability may be even close to one, that is, the spin-flipping and spin-conserving jumps may be almost equally frequent! Although an electron jumping into a spin hot spot is a rare event, it may nevertheless dominate the spin relaxation.

The above picture solves a longstanding experimental puzzle formulated first by Monod and Beuneu:[7] Why spin in some metals decays unexpectedly fast? Experiments show that alkali and noble metals have spin relaxation times consistent with the predictions of the theory of Elliott[8] and Yafet,[9] when the spin-flip rates are calculated from the atomic state parameters. Metals Al, Pd, Mg, and Be, on the other hand, have spin relaxation times much smaller (up to 3 orders of magnitude for Mg and Be) than estimated. This discrepancy is disturbing since it shows that otherwise similar metals may have very different spin relaxation times. Silsbee and Beuneu[10] were first to notice that accidental degeneracy points can significantly increase the spin relaxation of aluminum. We substantiated this idea by a rigorous calculation, and extended it to include all band-structure degeneracies. The experimental puzzle is then resolved by recognizing the fact that the two groups of metals have different valency. Alkali and noble metals are monovalent—their Fermi surface lies completely within the first Brillouin zone. The spin-flip rates are more or less uniform with the values close to the ones derived from atomic physics (there are no spin hot spots). On the other hand polyvalent Al, Pd, Mg, and Be have numerous Fermi surface anomalies where spin hot spots can be formed. Aluminum, for example, have spin relaxation rates determined primarily by the Fermi surface regions near the Brillouin zone boundaries and around the accidental degeneracy points.[6,10] In beryllium, the Fermi surface cuts through a degeneracy plane!

Since no polyvalent metals other than Al, Pd, Mg, and Be have been measured for T_1 so far, our explanation of the experimental puzzle becomes a prediction for future T_1 measurements. In addition, the spin-hot-spots picture suggests a way of altering T_1 via band-structure modifications. Doping into the conduction band, for example, may shift the Fermi surface away from some special symmetry points and increase T_1. Similarly, alloys or systems with reduced dimensionality will have spin relaxation rates different from those of the corresponding elemental or bulk metals, respectively. A general rule of thumb for increasing T_1 of electrons in a conduction band is washing out the spin hot spots from the Fermi surface. In what follows we introduce the basic concepts of our theory and discuss the results in a qualitative fashion.

If the periodic potential due to ions in a crystal lattice contains spin-orbit coupling (a term proportional to the scalar product of the orbital and spin momentum operators, $\hat{\mathbf{L}}\cdot\hat{\mathbf{S}}$), the electronic Bloch states are a mixture of spin up $|\uparrow\rangle$ and down $|\downarrow\rangle$ species:[8]

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$$\Psi^{\uparrow}_{\mathbf{k}n}(\mathbf{r})=[a_{\mathbf{k}n}(\mathbf{r})|\uparrow\rangle+b_{\mathbf{k}n}(\mathbf{r})|\downarrow\rangle]\exp(i\mathbf{k}\cdot\mathbf{r}), \tag{1}$$

$$\Psi^{\downarrow}_{\mathbf{k}n}(\mathbf{r})=[a^{*}_{-\mathbf{k}n}(\mathbf{r})|\downarrow\rangle-b^{*}_{-\mathbf{k}n}(\mathbf{r})|\uparrow\rangle]\exp(i\mathbf{k}\cdot\mathbf{r}). \tag{2}$$

The lattice momentum and band index are $\mathbf{k}$ and n, respectively, and $a_{\mathbf{k}n}(\mathbf{r})$ and $b_{\mathbf{k}n}(\mathbf{r})$ are complex periodic functions with the period of the lattice: if $\mathbf{G}$ denotes the reciprocal lattice vectors, then $a_{\mathbf{k}n}(\mathbf{r})=\Sigma_{\mathbf{G}}a_{\mathbf{k}n}(\mathbf{G})\exp(i\mathbf{G}\cdot\mathbf{r})$ and similarly for $b_{\mathbf{k}n}(\mathbf{r})$. Both states have the same energy $E_{\mathbf{k}n}$, as follows from time and space inversion symmetry;[8] the numbering of bands is therefore the same as without the spin notation. The degenerate states $\Psi^{\uparrow}_{\mathbf{k}n}$ and $\Psi^{\downarrow}_{\mathbf{k}n}$ are chosen to represent electrons with spins polarized along z direction:[9] $(\Psi^{\downarrow}_{\mathbf{k}n}|\hat{S}_z|\Psi^{\downarrow}_{\mathbf{k}n})=-(\Psi^{\uparrow}_{\mathbf{k}n}|\hat{S}_z|\Psi^{\uparrow}_{\mathbf{k}n})<0$ and the off-diagonal matrix elements are zero. This condition implies that $a_{\mathbf{k}n}(\mathbf{r})$ have values close to one, while $b_{\mathbf{k}n}(\mathbf{r})$ are much smaller, decreasing with the decrease of the strength of the spin-orbit interaction (with the exception of the points where the spin-orbit interaction lifts a degeneracy).

Elliott[8] pointed out that ordinary (spin conserving) impurity or phonon scattering can induce transitions between $\Psi^{\uparrow}_{\mathbf{k}n}$ and $\Psi^{\downarrow}_{\mathbf{k}'n'}$ (either their spin up or down amplitudes), leading to the flip of a spin polarization and thus spin relaxation. Simplifying assumptions lead to the formula[6]

$$1/T_1\approx 4\langle b^2\rangle/\tau, \tag{3}$$

where $\langle b^2\rangle$ is the Fermi surface average of

$$|b_{\mathbf{k}n}|^2=\sum_{\mathbf{G}}|b_{\mathbf{k}n}(\mathbf{G})|^2, \tag{4}$$

and τ is the momentum relaxation time. The weakness of the spin-orbit interaction makes the average spin-mixing parameter $\langle b^2\rangle$ much smaller than one and $1/T_1\ll 1/\tau$. At low temperatures, in a very pure sodium, for example, T_1 can reach a microsecond,[11] much larger than momentum relaxation times which would reach a fraction of a nanosecond in similar samples. Note that Eq. (3) implies a series "spin resistor" model (scattering rates are additive) for the spin relaxation, if $|b_{\mathbf{k}n}|^2/\tau$ is interpreted as the spin-flip rate for the scattering from, or to state $\mathbf{k}n$. The reason is that because $1/T_1\ll 1/\tau$, a single electron experiences many different ("series") scattering events before changing its spin. Therefore the Fermi surface states with the highest spin-flip rates count most. (A counterexample is conductivity which is monopolized by the states with the lowest scattering rates.)

In addition to the Elliott's mechanism, impurities and phonons affect the spin relaxation in other ways. Impurities induce the spin-orbit interaction which allows a direct transition between the spin up part of $\Psi^{\uparrow}_{\mathbf{k}n}$ and the spin down part of $\Psi^{\downarrow}_{\mathbf{k}'n'}$. The resulting spin relaxation is independent of temperature (as is the Elliot's impurity relaxation) and can be experimentally controlled. Similar transitions can be induced by the phonon-modulated spin-orbit interaction. This intrinsic effect leads, in principle, to a spin relaxation that is as effective as the Elliott's phonon-induced spin relaxation, but as we show below, becomes unimportant in many polyvalent metals where the Elliott's mechanism is enhanced by band structure.

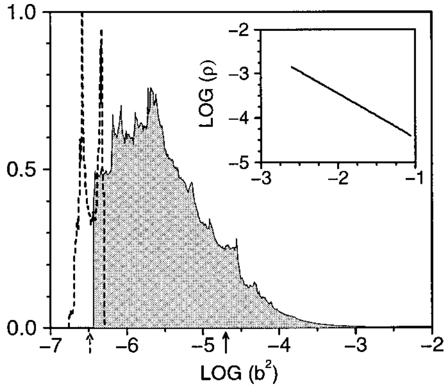

FIG. 1. Calculated distribution ρ (in arbitrary units) of the spin-mixing parameters $|b_{\mathbf{k}n}|^2$ for aluminum. The corresponding average $\langle b^2\rangle\approx 2.0\times 10^{-5}$ is indicated by a solid arrow. The linear tail of the distribution is shown in the inset. The dashed line shows what the distribution would be if aluminum were monovalent ($\langle b^2\rangle\approx 3.4\times 10^{-7}$, dashed arrow).

In most cases the spin-orbit interaction can be incorporated into the band structure as a perturbation, leading to the estimate $\langle b^2\rangle\approx(\lambda/\Delta)^2$. Parameter λ is some effective spin-orbit coupling and Δ is a typical (unperturbed) energy difference between neighboring bands. Monod and Beuneu[7] estimated both λ and Δ from their atomic values and found widely varying results for different metals. While this atomic substitution works well for alkali and noble metals, other metals (Al, Pd, Mg, and Be) seem to have $\langle b^2\rangle$ much larger than calculated. The case of aluminum and sodium is instructive. These metals have similar atomic numbers so their atomic λ/Δ are also similar (within 10%).[7] Yet their spin relaxation times differ by two orders of magnitude.[6,12–15] The reason is the very different band structure of the two metals that gives very different values for Δ. In sodium, Δ is of order E_F, the Fermi energy. In aluminum, Δ varies between zero (here perturbation theory for degenerate states gives $|b^2_{\mathbf{k}n}|\approx 0.5$) and E_F. Remarkably, the regions with small Δ (the spin hot spots) have enough weight to significantly increase the average $\langle b^2\rangle$ beyond the naive estimate $(\lambda/E_F)^2$ which works so well for monovalent metals. A solid state environment greatly influences $\langle b^2\rangle$ and T_1, leading to what we call the *band renormalization* of the spin-orbit mixing $\langle b^2\rangle$.

Figure 1 shows our calculation[6] of the distribution ρ of the values attainable by $|b_{\mathbf{k}n}|^2$ over the Fermi surface of aluminum. The width of the distribution is impressive—almost 7 decades! Most states have $|b_{\mathbf{k}n}|^2$ below 10^{-5}. Higher values are much less frequent but they stretch up to about 10^{-1} (we lacked enough precision to reach the upper limit 0.5) with ρ decreasing linearly, as seen in the inset. This long tail, however, has a marked influence on the average $\langle b^2\rangle\approx 2.0\times 10^{-5}$ which is an order of magnitude larger than the value where ρ is maximal. The unusual character of the distribution is further emphasized by the plot (also in Fig. 1) of ρ for a hypothetical case of monovalent aluminum. The band structure parameters (like the lattice structure or the form of the electron-ion potential) are unchanged so that any difference in ρ between the two metals is caused solely by their different valencies, and therefore different Fermi surface geometries. The distribution of b^2 is now relatively narrow with the average $\langle b^2\rangle \approx 3.4\times 10^{-7}$ coinciding with the center of the distribution; this value is about 50 times smaller than the average for (trivalent) aluminum. Adjusting for the density of states (monovalent aluminum would have $1/\tau$ reduced $\approx 3^{1/3}$ times) the spin relaxation would be about 70 times slower. This is about the measured difference between sodium, which has similar Fermi surface as monovalent aluminum, and aluminum.[6]

The difference between the two very different forms of ρ in Fig. 1 is clearly attributed to the subtleties of the band structure of aluminum. The Fermi surface of monovalent aluminum is nearly spherical and lies entirely within the first Brillouin zone; the protuberances near the zone boundaries do not touch the planes as in the case of the noble metals. On the other hand, the Fermi surface of aluminum crosses the Brillouin zone boundaries and accidental degeneracy lines.[16] The distorted electronic states near the crossings are responsible for the long tail of ρ. Consider a band structure computed without the spin-orbit interaction. The spin-orbit interaction, being a part of the periodic lattice potential can induce transitions only between states whose **k** differ by a reciprocal lattice vector, or, in a reduced-zone scheme, between the states with the same **k** but different n. Let, for a state $\mathbf{k}n$ on the Fermi surface, the closest band to n is separated from n by Δ. The spin-orbit interaction mixes the spin amplitudes from the two bands (more distant bands to n will have smaller contribution and we neglect them) leading to the spin-mixing parameter $|b_{\mathbf{k}n}|^2 \approx (1-\Delta/\sqrt{\Delta^2+4\lambda^2})/2$. Three cases can occur. (A) For a general point on the Fermi surface, the band separation is of order E_F, the Fermi energy, so that $\Delta \gg V_{\mathrm{SO}}$ and $|b_{\mathbf{k}n}|^2 \approx (V_{\mathrm{SO}}/E_F)^2$. This is the case of monovalent aluminum: parameters $\lambda \approx 3$ meV (same as for trivalent aluminum)[6] and $E_F \approx 6$ meV give $|b_{\mathbf{k}n}|^2 \approx 3\times 10^{-7} (\approx 10^{-6.6})$ in accordance with Fig. 1. In (trivalent) aluminum typical spacings between bands are somewhat smaller than $E_F \approx 12$ eV; the estimate of $\Delta \approx 3$ eV is in reasonable agreement with Fig. 1. (B) If the state is close to a Brillouin zone boundary associated with **G**, the band separation is $\approx 2V_{\mathbf{G}}$ ($V_{\mathbf{G}}$ is the **G**th Fourier coefficient of the nonspin part of the lattice potential). Since typically $V_{\mathbf{G}} \gg V_{\mathrm{SO}}$, $|b_{\mathbf{k}n}|^2 \approx (V_{\mathrm{SO}}/2V_{\mathbf{G}})^2$; this can be a few orders larger than in (A). Aluminum has $V_{111} \approx 0.2$ eV which gives $|b_{\mathbf{k}n}|^2$ about $6\times 10^{-5} (\approx 10^{-4.2})$ coinciding with the onset of the tail in Fig. 1. Curiously, the Fermi surfaces of the noble metals too come in contact with some zone boundaries. The noble metals, however, have unusually large $V_{\mathbf{G}}$[17] so the estimate (A) works equally well. Finally, (C) the spin-orbit interaction can lift the degeneracy of two or more bands. The mixing of spins is complete and $|b_{\mathbf{k}n}|^2 \approx |a_{\mathbf{k}n}|^2 \approx 0.5$. Even this case occurs in aluminum, where the second and third band accidentally coincide at some Fermi surface points (the accidental degeneracy points). The neighborhood of these points is responsible for the long tail of ρ in Fig. 1. The spin hot spots are the states with the properties (B) and (C).

As Fig. 1 reveals, the spin hot spots essentially determine the average $\langle b^2\rangle$. We give a simple example demonstrating that this is reasonable. Consider electrons in the presence of a single Brillouin zone plane that is associated with the reciprocal vector **G**. If the electron-ion potential (or, rather, pseudopotential) is weak, the band structure of such a system is found by using just two plane waves, $\exp(i\mathbf{k}\cdot\mathbf{r})$ and $\exp[i(\mathbf{k}-\mathbf{G})\cdot\mathbf{r}]$; this is sometimes known as the two orthogonalized-plane-wave (OPW) method.[18] The problem has axial symmetry along the direction of **G**, so we conveniently shift the origin of **k** to **G**/2 and decompose **k** into the components parallel (**z**) and perpendicular (**r**) to **G**: $\mathbf{k}=\mathbf{G}/2+\mathbf{r}+\mathbf{z}$. To further simplify the notation, energy and momentum will have the units of $\hbar^2(G/2)^2/(2m)$ and $G/2$, respectively; m will be the electron mass. The band structure is formed by two energy levels with the dispersion (see, for example, Ref. 18)

$$E^{\pm} = 1 + r^2 + z^2 \pm \tfrac{1}{2}\,\mathrm{sgn}(z)\Delta(z), \tag{5}$$

$$\Delta(z) = \sqrt{16z^2 + 4V_{\mathbf{G}}^2}. \tag{6}$$

We allow z which measures the distance from the plane, both negative and positive values (repeated-zone scheme) and take E^+ as the reference level. The Fermi surface is then the revolution of the curve

$$E^{+}(r,z) = E_F \tag{7}$$

about **G**. If z is negative (states inside the first Brillouin zone) E^- is the upper band, if z is positive E^- is smaller than E^+; the spacing between the two bands $\Delta(z)$ depends only on z.

The spin-orbit interaction will mix the spin amplitudes of the two bands. In most cases $\lambda \ll V_{\mathbf{G}}$ and we can use the estimate (B):

$$|b_{\mathbf{k}n}|^2 \equiv |b_z|^2 \approx [\lambda/\Delta(z)]^2. \tag{8}$$

A proper evaluation of $|b_{\mathbf{k}n}|^2$ would, instead of effective λ, have the matrix elements of the spin-orbit interaction between the band states with energies E^- and E^+. Such matrix elements, in general, depend on both r and z, and for spin quantized not along **G**, also on the angle of revolution ϕ. In particular, the spin mixing would vanish at $\mathbf{k}=\mathbf{G}/2$ (that is, $r=z=0$). This follows from group-theoretical arguments[19] or, more simply, from the fact that the spin-mixing matrix elements between the plane waves $\exp(i\mathbf{k}\cdot\mathbf{r})$ and $\exp[i(\mathbf{k}-\mathbf{G})\cdot\mathbf{r}]$, out of which the band states are formed, are proportional to the vector product $\mathbf{k}\times(\mathbf{k}-\mathbf{G})$; this product vanishes for $\mathbf{k}=\mathbf{G}/2$. Incidently, this vanishing of spin mixing is another reason why the band structure does not affect T_1 for the noble metals despite the fact that some of their states come into contact with zone boundaries at **G**/2. Introducing effective λ therefore overestimates the region around **G**/2. In most interesting cases of polyvalent metals, however, the Fermi surface crosses the plane far enough from this point (that is, if $z=0$ radius r is a significant fraction of $G/2$) and our approach is justified.

The Fermi surface average of $|b_z|^2$ given by Eq. (8) is

$$\langle b^2\rangle = \frac{1}{z_2 - z_1}\int_{z_1}^{z_2} dz\,\frac{\lambda^2}{\Delta^2(z)}. \tag{9}$$

The limits of the integration, z_1 and z_2, are the minimum and maximum value of z reached by the Fermi surface; they

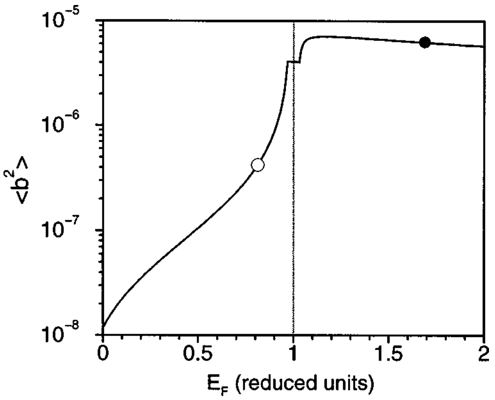

FIG. 2. Two OPW calculation (with the parameters V_G and λ suitable for aluminum) of the average spin-mixing parameter $\langle b^2\rangle$ as a function of the Fermi energy E_F. The values of $\langle b^2\rangle$ that correspond to monovalent (open circle, $E_F=0.81$) and trivalent (filled circle, $E_F=1.7$) aluminum are 4.1×10^{-7} and 6.2×10^{-6}, respectively. The vertical line indicates the case where the free-electron Fermi sphere comes into contact with the Brillouin zone boundaries.

are obtained by putting $r=0$ and solving Eq. (7) for z. We are interested in how $\langle b^2\rangle$ depends on the Fermi surface geometry. The Fermi energy which determines z_1 and z_2 will now be a variable parameter (simulating doping). Although the integral in Eq. (9) can be evaluated analytically it is more instructive to consider some limiting cases only. The numerical estimates will be done with the band-structure parameters appropriate for aluminum so that the results can be directly compared with the full band structure calculation of Fig. 1. The parameters are $\lambda\approx 4.3\times 10^{-4}$ and $V_{\mathbf{G}}=V_{111}\approx 0.035$ (we now use the dimensionless units for energy). Although the aluminum Fermi surface crosses both (111) and (200) zone boundaries, we choose as $V_{\mathbf{G}}$ the Fourier coefficient V_{111} which is much smaller than V_{200} and has therefore greater impact on $\langle b^2\rangle$.

If E_F is small, the Fermi surface is a small, almost undistorted sphere. Both z_1 and z_2 are close to -1 so we can neglect $V_{\mathbf{G}}$ in Eq. (6) and obtain $\langle b^2\rangle\approx\lambda^2/16\approx 1.2\times 10^{-8}$. This number is not affected by the presence of the Brillouin zone boundaries and can be thought of as an atomic limit for the spin mixing. When E_F is large enough for the Fermi surface to cross the zone boundary, $z_2\gtrsim -V_{\mathbf{G}}$ and the small region of the states around the plane gives the dominant contribution to $\langle b^2\rangle$. Indeed, when taking the integral in Eq. (9) from $-V_{\mathbf{G}}$ to $V_{\mathbf{G}}$ only, $\Delta(z)\approx 2V_{\mathbf{G}}$ and $\langle b^2\rangle\approx\lambda^2/(4V_{\mathbf{G}}k_F)$; the Fermi momentum $k_F=\sqrt{E_F}$ is given by $z_2-z_1\approx 2k_F$. Before substituting numerical values we note that there are eight (111) planes in aluminum. They contribute independently to $\langle b^2\rangle$ giving the estimate $\langle b^2\rangle\approx 8\times 10^{-6}$. The full calculation in Fig. 1 gives the value which is more than twice larger. This is explained partly by our neglect of the (200) planes and, more important, by ignoring the accidental degeneracy points.

Figure 2 plots the full dependence of $\langle b^2\rangle$ on E_F within the two OPW approximation for the eight (111) aluminum planes. Doping, or increasing the size of the Fermi surface can increase $\langle b^2\rangle$ by almost 3 orders of magnitude. As the Fermi surface expands towards the zone boundaries, the Bloch states that are closest to the planes (they have smallest Δ) become more and more important. Once the Fermi surface reaches the plane (at the energy $1-V_{\mathbf{G}}\approx 0.97$) the average $\langle b^2\rangle$ goes through a maximum and then slightly decreases. The decrease is tied to the saturation of the integral in Eq. (9): only the states in the small neighborhood of the plane are dominant and $\langle b^2\rangle\sim 1/(z_2-z_1)$. The quantity z_2-z_1 is up to a numerical factor the density of states. As Fig. 1 shows, in this toy calculation monovalent aluminum would have $\langle b^2\rangle$ about 15 times smaller than aluminum, in good agreement with the results of Fig. 1.

The qualitative understanding of the above estimates for the impact of a Brillouin zone boundary on $\langle b^2\rangle$ is quite simple. We need to estimate the probability with which an electron in its random walk on the Fermi surface jumps into a state close to a Brillouin zone boundary. Alternatively, we can ask what is the portion of the free-electron Fermi surface states that have $\Delta\lesssim 2V_{\mathbf{G}}$ (these states will be significantly perturbed by the presence of the boundary). The answer is $\sim V_{\mathbf{G}}$ and the reason that this number is linear in $V_{\mathbf{G}}$ (the linearity is crucial) is that Δ increases linearly away from the plane, as in Eq. (6). The average value $\langle b^2\rangle$ is then $\sim V_{\mathbf{G}}\times\lambda^2/V_{\mathbf{G}}^2\approx\lambda^2/V_{\mathbf{G}}$. The enhancement of the spin mixing due to the presence of a single Brillouin zone boundary is then $\sim 1/V_{\mathbf{G}}$, as in Fig. 2.

To estimate how accidental degeneracy points affect $\langle b^2\rangle$ is more difficult.[10] Consider two bands coming into contact at a single point R, different from the symmetry points, on the Fermi surface. As noted in Ref. 18 the band spacing Δ grows linearly as we go away from R in almost all directions (the exception is the direction along the corresponding accidental degeneracy line). We need to divide the region around R in two: the first has states with $0\lesssim\Delta\lesssim 2\lambda$, the second with $2\lambda\lesssim\Delta\lesssim 2V_{\mathbf{G}}$. Since $\Delta\sim\delta k$, where δk measures the distance from R, there are $\sim\lambda^2$ points in the first region, all with (approximately) the same value of $b_{\mathbf{k}n}\sim 1$ from estimate (C). The average $\langle b^2\rangle$ therefore scales as λ^2. The second region is different in that we have $b_{\mathbf{k}n}$ depending on Δ [estimate (B)]. The average $\langle b^2\rangle$ is thus proportional to

$$\langle b^2\rangle\approx\int_{\lambda}^{V_G} d\Delta\,\Delta\,\frac{\lambda^2}{\Delta^2}. \tag{10}$$

This integral evaluates to $\lambda^2\ln(V_{\mathbf{G}}/\lambda)$ giving a weak enhancement of about $\ln(V_{\mathbf{G}}/\lambda)\approx 4$. More accurate evaluation based on a four OPW approximation would give an additional enhancement of $(V_{200}/V_{111})^2\approx 10$.[6] As $V_{\mathbf{G}}$ becomes smaller the importance of accidental degeneracy points diminishes.

Another type of a spin hot spot, not relevant for aluminum though, is the region around a special symmetry point. It may happen that the Fermi energy coincides with a set of two or more degenerate levels at a symmetry point. This is the case, for example, of the (fcc) palladium and platinum, whose Fermi surfaces go through the fcc L points.[20] If the spin-orbit interaction lifts this degeneracy, the renormalization of $\langle b^2\rangle$ can be significant. This effect is, however, not easy to estimate qualitatively. For the fcc W point we find that the enhancement of $\langle b^2 \rangle$ relative to the atomic value of $\sim \lambda^2$ is about $V_{\mathbf{G}}/\lambda$.[19] This can range from a 10 to a 1000.

Our final note concerns the hexagonal Mg and Be, where the deviation of T_1 from the simple estimates is most striking.[7] We argue that this is also a manifestation of the band renormalization of $\langle b^2 \rangle$. Without the spin-orbit interaction, all the states at the hexagonal faces of the first Brillouin zone of a simple hexagonal structure are degenerate.[21] The spin-orbit interaction lifts this degeneracy[8] (except at some symmetry points and lines), presumably by the amount $V_{\mathbf{G}}\lambda$, the largest second-order term containing the spin-orbit interaction (any first order term vanishes since the structure factor associated with the hexagonal faces is zero).[21] The contribution to $\langle b^2 \rangle$ of the points where the Fermi surface intersects the hexagonal faces is $\sim V_{\mathbf{G}}\lambda$: the characteristic value $|b_{\mathbf{k}n}|^2 \sim 1$, times the area of the affected part of the Fermi surface, $V_{\mathbf{G}}\lambda$. The enhancement measured in terms of λ^2 is then $V_{\mathbf{G}}/\lambda$; this can be as large as a thousand for light elements like Mg and Be.

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