TOPICAL REVIEW

Tunneling magnetoresistance from a symmetry filtering effect

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Abstract

This paper provides a brief overview of the young, but rapidly growing field of spintronics. Its primary objective is to explain how as electrons tunnel through simple insulators such as MgO, wavefunctions of certain symmetries are preferentially transmitted. This symmetry filtering property can be converted into a spin-filtering property if the insulator is joined epitaxially to a ferromagnetic electrode with the same two-dimensional symmetry parallel to the interface. A second requirement of the ferromagnetic electrodes is that a wavefunction with the preferred symmetry exists in one of the two spin channels but not in the other. These requirements are satisfied for electrons traveling perpendicular to the interface for Fe–MgO–Fe tunnel barriers. This leads to a large change in the resistance when the magnetic moment of one of the electrodes is rotated relative to those of the other electrode. This large tunneling magnetoresistance effect is being used as the read sensor in hard drives and may form the basis for a new type of magnetic memory.

Keywords: tunneling magnetoresistance, TMR, evanescent state, symmetry filter, complex energy band, delta-1 state, interfacial resonance states, magnetic tunnel junction

(Some figures in this article are in colour only in the electronic version.)

1. Spintronics

Tunneling magnetoresistance is one of several relatively new phenomena that have contributed to the growth of the young field of ‘spintronics’. Spintronics can be defined as the art and science of utilizing the spin of the electron (as well as its charge) to accomplish some purpose. The birth of spintronics can be dated from 1988 when groups led by Albert Fert and Peter Grünberg independently discovered the phenomenon of Giant Magnetoresistance (GMR) [1, 2]. Their contribution was recognized this year (2007) by the award of the Nobel Prize in physics.

This recognition is well deserved because their work caused a paradigm shift in the way we think about magnetic materials. Before their discoveries, magnetic materials were of interest because of the magnetic fields that they could create, the forces they could exert on nearby objects and their ability to retain information, e.g. in the direction of their magnetization. The discovery of GMR reminded us that ferromagnetic materials can be considered as two different materials simultaneously occupying the same space; the properties of one of these materials being determined by the electronic structure of the majority spin electrons and those of the other by the electronic structure of the minority spin electrons. Their work showed us how to make these two different personalities of a ferromagnet evident through the way they affect the transport of electrons.

The majority-spin and minority-spin electrons are sometimes referred to as ‘up’ or ‘down’ spin electrons, respectively.
1.1. Spintronic phenomena

There are now several types of spintronic phenomena. The most important are Giant magnetoresistance which appears in two basic versions (current in the plane and current perpendicular to the plane), tunneling magnetoresistance and spin-torque.

**Giant Magnetoresistance (GMR)** is a change in the resistance of a magnetically inhomogeneous material when an applied magnetic field brings the magnetic moments of the material into alignment. The magnetically inhomogeneous system usually consists of a magnetic multilayer in which the layers are typically a few nanometers in thickness. It is useful and customary to divide GMR into two major types, Current in the Plane (CIP) GMR and Current Perpendicular to the Plane (CPP) GMR. The physics of these two types of GMR are quite different. The type of GMR first observed by the teams led by Fert and Grünberg is CIP GMR.

In CPP GMR, the current is parallel to the planes of the layered magnetic film. Observation of CIP GMR requires at least two ferromagnetic layers separated by a thin metallic spacer layer. To observe GMR one contrives circumstances such that the magnetic moments in the ferromagnetic layers in the absence of an applied magnetic field are not aligned. On application of a sufficiently strong magnetic field, the moments are pulled into alignment and GMR manifests itself as a change in the in-plane electrical resistance. CIP GMR depends on the fact that electrical conduction is a non-local effect. Electrons may be accelerated by the electric field in one ferromagnetic layer and travel through the spacer layer where they contribute to the conductance in the second spacer layer. The alignment of the magnetic moments matters because when the moments are aligned, up-spin electrons in one ferromagnetic layer will be up spin-electrons in the second layer whereas if the moments are anti-aligned locally up spin-electrons in one layer will be locally down-spin when they drift into the second ferromagnetic layer.

One important contributor to both CIP and CPP GMRs is the matching of the electronic structures of the spin-channels. For example, the first observation of GMR was in Fe–Cr multilayers. It turns out that Fe and Cr have very similar minority spin bands whereas their majority spin bands are quite different. An important type of spin-valve used in magnetic field sensors is based on layers of Cu and Co (or materials similar to Co in the majority channel). The electronic structure of Cu is rather similar to the electronic structure of majority spin Co. There can be other important contributors to CIP GMR including a ‘wave guide’ effect that causes channeling of electrons within the Cu layer [3].

CPP GMR is conceptually simpler than CIP GMR. It can be understood even within a local picture of conduction. However, it is probably more difficult to treat quantitatively. In CPP GMR the electrons travel perpendicular to the magnetic layers. It is relatively easy to see in a qualitative picture how if the majority or minority bands of the two ferromagnetic layers match the spacer layer, electrons in one of the spin channels can easily pass through the layers when the moments are aligned. Furthermore, some magnetic alloys, e.g. Ni-rich alloys containing Co and Fe conduct up spin electrons with very little scattering while down spin electrons can hardly travel more than an interatomic distance before they scatter.

CPP GMR is difficult to measure because the resistance of a thin film (thickness measured in tens of nanometers versus cross section in square micrometers) is usually tiny across its thickness. The thickness must remain small compared to the distance over which the electrons remember their spin which for magnetic materials is on the order of one to twenty nanometers. For this reason, the first CPP-GMR measurements were performed using superconducting leads [4]. The first major application of CPP-GMR will probably be extremely small magnetic field sensors (~10 nm), so small that their lateral dimensions are comparable to the film thickness.

**Tunneling Magnetoresistance (TMR)** is geometrically similar to CPP-GMR. The difference is that the non-magnetic metallic spacer layer is replaced by an insulator or semiconductor. It would appear that band-matching between one of the spin-channels and the spacer layer (the origin of CPP GMR) can no longer occur because there are no bands at the Fermi energy in an insulator. For this reason (as will be described below) the theory of TMR was based on the Fermi energy density of states of the ferromagnetic electrodes. Somewhat surprisingly, as will also be described below, it turns out that a new and different kind of band matching can occur and this can be used to achieve a very large ratio of tunneling conductance between parallel and anti-parallel alignment of the spins.

**Spin-Torque** is the newest major spintronic phenomenon. It was predicted independently by John Slonczewski and Luc Berger in 1996 [5, 6]. In a sense, it is the converse of GMR and TMR in which the transport of electrons between two ferromagnetic layers is affected by the relative alignment of their magnetic moments. It is probably not surprising that currents flowing between ferromagnetic layers can change the relative alignment of their magnetic moments. Spin-polarized currents have been observed to cause precession of magnetic moments and switching from anti-parallel to parallel relative alignment and vice versa.

1.2. Spintronic applications

**1.2.1 Read sensors for hard drives.** The CIP-GMR spin valve was the first major application of spintronics. These devices have been used since the mid-1990s to detect the
transitions between the magnetic domains which encode the information stored on hard drives. The size of a read sensor in a hard drive must be comparable to the bit size. One of the major advantages of the GMR spin-valve is that it allowed the sensor to decrease in size keeping pace with (and enabling) the rapidly decreasing size of the magnetic bit as storage densities have increased. In a CIP spin-valve, the moments of one of the ferromagnetic layers (called the ‘pinned’ or ‘reference’ layer) are held in a fixed direction by means of an adjacent anti-ferromagnetic layer whose local moments are tightly coupled to those of the ferromagnetic layer. The other ferromagnetic layer (called the ‘free’ layer) is designed so that it will respond to an applied field. Various schemes are used to ensure that in the absence of an applied field, the moments of the ‘free’ layer are oriented perpendicular to the moments of the pinned layer. This is done to ensure a linear response of the resistance to the applied field. CIP-GMR spin-valves rapidly became the dominant technology for hard drive read sensors in the late 1990s.

**TMR read sensors** have recently displaced the CIP-GMR spin valve as the dominant technology for hard drives because they are easier to fabricate at smaller sizes than CIP-GMR devices and because they can provide a much larger signal. Because of the design of the read/write head, it is easier to make a small read sensor if the current flows perpendicular to the layers. The recent prediction, discovery and development of symmetry filter based TMR sensors (described below) has made it possible to obtain a large signal from a very small TMR device with a resistance that is not so high that shot noise becomes a problem.

As bit sizes continue to decrease it is expected that even the new class of TMR sensors will encounter the shot-noise problem. Shot noise arises because the electronic charge is discrete. As tunnel devices are made smaller and smaller, and the total current becomes smaller, there will be random fluctuations in the current as the electrons tunnel through the barrier at random times. When shot noise becomes too large, it is expected that CPP-GMR based spin-valves may become the preferred technology. It should be possible to make CPP-GMR devices that show an extremely large change in resistance between parallel and anti-parallel alignment of the magnetic layers using materials called half-metals. Half-metals are metals for one spin-channel, but insulators (or semiconductors) for the other spin-channel.

### 1.2.2 Magnetic random access memory

TMR is also used to read the information stored in a new type of non-volatile magnetic memory called Magnetic Random Access Memory (MRAM). In principle MRAM has many advantages over current alternatives. It can be relatively fast (especially if it takes advantage of the large signal offered by symmetry based TMR), it is non-volatile which gives it an advantage over conventional dynamic random access memory which requires refreshing and it offers an unlimited number of read and write cycles. Compared to flash memory, MRAM has the advantages of unlimited read and write cycles and much shorter write times. The advantage of flash is that of a more mature technology which can be made quite dense and is presently much less expensive per bit.

In MRAM the information is stored in the relative orientation of two magnetic layers. Parallel orientation might represent a zero, anti-parallel might represent a one. TMR is used to sense the difference in resistance of the two states. One difficulty with scaling MRAM to smaller bit sizes and higher densities is its mechanism for writing which uses magnetic fields supplied by current carrying lines to switch the moments of one of the layers, i.e. the free layer relative to a pinned layer. A possible solution to this problem that is being aggressively explored is to utilize spin-torque for switching the moments of the free layer.

#### 1.2.3 Other applications

GMR and TMR can be used wherever there is a need for an electrical response to a magnetic field. They are particularly appropriate when the sensors need to be small or where an array of sensors is needed.

It has been suggested [8, 9] that MRAM-type cells with very large ratios of parallel to anti-parallel conductance might enable a new type of computer architecture in which logic circuits are reprogrammed dynamically. Such a device would be similar to a field programmable gate array that could be reprogrammed on a nanosecond timescale.

One major goal of current research in spintronics is to electrically generate and manipulate spin-polarized currents in semiconductors. The symmetry filter effect can, in principle, be used to inject strongly spin-polarized currents into semiconductors such as GaAs. These should be particularly long lived if they are injected into the conduction band because of the weak spin–orbit coupling near the bottom of the conduction band of a typical semiconductor such as GaAs. Transistors based on the precession of spins injected into semiconductors have been proposed, but so far have not been realized [10]. Another possible direction for future spintronic research is the use of low Z and high conductivity materials such as carbon nanotubes and graphene for conducting spin-polarized currents. The transmission of spin-polarized currents over micron length scales has been demonstrated in carbon nanotubes [11].

### 2. Tunneling Magnetoresistance

Tunneling magnetoresistance was first reported by Julliere in 1975 [12]. Julliere made a Co–Ge–Fe sandwich and measured the change in electrical resistance on switching the relative alignment of the Co and Fe magnetic moments from parallel to anti-parallel. He reported a 14% increase in resistance at a temperature of 4.2 K. This short paper is also famous for the introduction of the Julliere model for TMR which continues to be the most often used theory for analyzing the results of TMR experiments. Julliere’s work may have been inspired in part by the work of Tedrow and Meservey [13, 14] who had earlier measured the spin-dependence of tunneling currents through an amorphous aluminum oxide tunnel barrier separating various ferromagnetic electrodes from superconducting aluminum. After the discovery of GMR
in 1988, tunneling magnetoresistance received much more attention. In 1995 Miyazaki et al. [15] and Moodera et al. [16] independently reported TMR in excess of 10% at room temperature. This was sufficient to make TMR interesting for applications.

During the 1970s there was considerable interest in quantum mechanical tunneling between metallic electrodes in which at least one of the leads was a superconductor. It was learned during this period that aluminum oxide makes an excellent tunnel barrier. The probable reason for this is that aluminum has a remarkable affinity for oxygen. The aggressive oxidation process leads to amorphous but highly coherent oxides that give complete coverage without pinholes even when the layers are very thin. These thin aluminum oxide layers are very important for tunneling. The many orders of magnitude difference in the conductivity of the metal and the oxide mean that even a small number of pinholes will dominate the measured conductance. On the other hand the oxide cannot be very thick. The resistance of a tunneling device increases very rapidly with thickness, even when the layers are very thin. These thin aluminum oxides that give complete coverage without pinholes were learned during this period that aluminum oxide makes synonymous with amorphous aluminum oxide barriers.

2.1. Two current model

Descriptions of spintronic effects are typically based on the ‘two current model’ of electron transport in solids [17]. Within this model, the up-spin and down-spin electrons conduct in parallel. Consider the tunneling conductance between two ferromagnetic electrodes. Within the two-current model, the conductance for the cases of parallel and anti-parallel alignment of the magnetic moments of the electrodes are written as \( G_P = G^\uparrow \uparrow + G^\downarrow \downarrow \) and \( G_{AP} = G^\uparrow \downarrow + G^\downarrow \uparrow \), respectively. Thus for parallel alignment of the electrodes the up-spin electrons on the left side are still up-spin on the right after tunneling through the barrier. Similarly, the down-spin electrons on the left remain down-spin on the right. For anti-parallel alignment, however, electrons that are locally up spin (meaning their moment is parallel to that of the local magnetization) find themselves in a region of opposite magnetization which means that they are locally down-spin. Similarly, down spins on the left become up spins on the right.

The two-current model neglects the spin–orbit interaction, a relativistic effect that couples the electron’s spin with its orbital motion around the nucleus and through the lattice. It also neglects the possibility that there may be magnetic moments (especially near the interfaces) that are not perfectly aligned with those of their layer. Imperfect alignment can occur because of thermal effects or because of weak exchange interactions. Exchange interactions are the name we give to the quantum mechanical effect that causes the magnetic moments in ferromagnets to align in a common direction.

2.2. Julliere model

In his short, but famous 1975 paper, Julliere explained his results using a simple and easily applied theory that will be described here. Julliere proposed that the tunneling current should be proportional to the density of electronic states on the transmitting side of the barrier and to the density of electronic states on the receiving side of the barrier. This proposal may seem reasonable since transition probabilities are often proportional to the densities of initial and final states. There are also matrix elements involved in transition probabilities, but those are difficult to calculate for a barrier like AlO\(_x\) so the effect of the matrix element was incorporated into the density of states through the notion that the density of states being described was ‘the density of states of the tunneling electrons’. Presumably, some electrons can tunnel more easily than others.

If we ignore the ambiguity in what is meant by ‘density of states’ in the Julliere approach, it is straightforward to derive a simple formula for TMR. The equations, \( G_P = G^\uparrow \uparrow + G^\downarrow \downarrow \) and \( G_{AP} = G^\uparrow \downarrow + G^\downarrow \uparrow \) mathematically express the parallel conductance implied by the two current model for the case of parallel and anti-parallel alignment of the moments of the two electrodes, respectively. The hypothesis that the conductance is proportional to the density of states of the left and right electrodes implies,

\[
G^\uparrow \downarrow \propto N_L^\uparrow N_R^\downarrow, \quad G^\downarrow \uparrow \propto N_L^\downarrow N_R^\uparrow, \quad G^\uparrow \uparrow \propto N_L^\uparrow N_R^\uparrow, \quad G^\downarrow \downarrow \propto N_L^\downarrow N_R^\downarrow.
\]

Defining the tunneling magnetoresistance as the ratio of the change in conductance to the minimum conductance, we have,

\[
\text{TMR} = \frac{G_P - G_{AP}}{G_{AP}} = \frac{N_L^\uparrow N_R^\downarrow + N_L^\downarrow N_R^\uparrow - N_L^\uparrow N_R^\uparrow - N_L^\downarrow N_R^\downarrow}{N_L^\uparrow N_R^\uparrow + N_L^\downarrow N_R^\downarrow}.
\]

Defining the polarization of the left and right electrodes by

\[
P_{LR} = \frac{N_L^\uparrow N_R^\downarrow - N_L^\downarrow N_R^\uparrow}{N_L^\uparrow N_R^\uparrow + N_L^\downarrow N_R^\downarrow} = \frac{\Delta N_{LR}}{N_{LR}},
\]

we obtain

\[
\text{TMR} = \frac{2P_{LR}P_R}{(1/2)(N_L N_R - \Delta N_L \Delta N_R)} = \frac{2P_{LR}P_R}{1 - P_L P_R}.
\]

Thus the TMR is expressed in terms of the ‘spin-polarization’ of the left and right electrodes. Although this formula is much used to rationalize TMR experiments and often seems to be useful for this purpose, its meaning is not so clear as our simple derivation appears to imply. The polarization, \( P_{LR} \), cannot be interpreted as the polarization of the density of states at the Fermi energy as implied in the derivation. The reason for this is that the spin polarization of the tunneling current can be measured when electrons tunnel between a ferromagnetic electrode and a superconducting electrode. For Co and Ni which are known to have a Fermi energy density of states that is overwhelmingly minority, it is the majority electrons that are observed to carry the tunneling current in these experiments. Another indication that the TMR depends not just on the barrier but also on the electrodes is that the sign of the TMR has been observed to change when the barrier is changed using the same electrode materials [18].
The Julliere formula is most appropriate when comparing TMR for systems with different electrode materials but identical barriers. When almost all barriers were AlO, this was quite useful. The free electron—simple barrier model for quantum mechanical tunneling (described in the next section) can be solved analytically. The TMR is not given by the Julliere model if the polarizations are defined in terms of the density of states at the Fermi energy. However, the TMR can be expressed in the Julliere form if the polarizations are defined in terms of the probabilities for up- and down-spin electrons in one of the electrodes to be ‘transmitted’ into the barrier as an evanescent wave [19]. In general, however, it must be admitted that there is not yet a good theory of TMR for systems with amorphous barriers.

### 2.3. Theory of tunneling in epitaxial systems

Let us now consider tunneling for epitaxial systems. Fortunately, relatively straight-forward theoretical approaches exist for such systems. A simple and effective approach for understanding and calculating ballistic transport was developed by Landauer [20]. In this approach one imagines (figure 1) two reservoirs of electrons, one on the left at chemical potential $\mu_1$ and another on the right at chemical potential $\mu_2$. At $T = 0$, electrons with energies less than $\mu_1$ in the left reservoir contribute to an electron current that flows from left to right while electrons in the right reservoir with energies less than $\mu_2$ contribute to an electron current in the opposite direction. The difference between these currents will be the net current flowing through the sample for applied bias, $V = (\mu_1 - \mu_2)/e$.

#### 2.3.1 Landauer expression for tunneling conductance

The current density for right going electrons in the left lead can be written as, $J^+ = \frac{e}{V} \sum \psi^*(k) f(\mu_1)$. Here, the volume $V$ is the cross-sectional area $A$ times some length $l$ along the lead. Note that we are including all of the electrons from some minimum energy up to the local chemical potential. Note also that we are only counting the electrons whose velocity in the $z$-direction is positive. In equilibrium, ($\mu_1 = \mu_2$) there will be an equal number of electrons at each energy going in the opposite direction so the net current density would be zero. The sum over wavevectors consists of a sum over $k_z$ to the corresponding integral, $\sum k_z \rightarrow \frac{1}{2\pi} \int dk_z$, to convert the sum over $k_z$ into an integral,

$$J^+ = \frac{e}{A} \sum_{k_z} \frac{1}{2\pi} \int \frac{1}{h} \frac{\partial E(k)}{\partial k_z} f(\mu_1) \sum_{k'} T^{++}(k, k').$$

Multiplying $J^+$ by the area to get $I^+$, we obtain,

$$I^+ = \frac{e}{h} \sum_{k_z} \int dk_z \frac{\partial E(k)}{\partial k_z} f(\mu_1) \sum_{k'} T^{++}(k, k').$$

We also included the probability that the electron will be transmitted through the sample region to states $k'$ in lead 2. We can now convert the integral over $k_z$ into an integral over energy, obtaining an expression for $I^+$, the current of electrons, in the left lead being transmitted to the right,

$$I^+ = \frac{e}{h} \int dE \sum_{k_z} T^{++}(k, k').$$

A similar procedure yields the corresponding expression for $I^-$, the current of electrons in the right lead being transmitted to the left,

$$I^- = \frac{e}{h} \int dE \sum_{k_z} T^{--}(k, k').$$

The difference of these two currents gives the net current through the sample and for small differences between the
Figure 3. Energy bands in MgO along the (100)-direction. The red, green and blue bands were calculated for MgO. The black band represents the simple barrier model with free electron mass.

Figure 4. Plot of $(k_z, \Delta z)^2$ versus energy showing how one of the valence bands (red) continues as an evanescent state into the gap and then becomes the conduction band. The black line gives $(k_z, \Delta z)^2$ for the simple barrier model. For the bands shown here $k_\parallel$ was set to zero. One Hartree is 27.2 eV.

Figure 5. Simple model for the $\Delta_1$ valence and conduction bands of MgO. The simplified Hamiltonian includes the magnesium s-state represented by the blue circles and the oxygen $p_z$ state indicated by the red ($\psi < 0$) and green ($\psi > 0$) ellipses.

Figure 6. Energy as a function of wavevector for $\Delta_1$ bands in MgO. The red lines are the results of first-principles calculations using DFT. The blue dotted lines result from the simple two orbital approximation described above.
In this review, I will contrast the simple barrier model with a more realistic model that results when one includes the atoms that make up the electrodes and barrier. Understanding the barrier model, however, makes it easier to understand some of the results of the more realistic models.

In the barrier model, one envisions free electrons with energy $E$ propagating in some direction determined by the wavevector $\mathbf{k}$, incident on a barrier of height $V$ (greater than $E$) that extends from $z = 0$ to $z = t$. The barrier is assumed to have infinite extent in $x$ and $y$. In this case, of electrons incident from $z = -\infty$, the $x$-component of the wavevector is assumed to be positive. This problem can be solved analytically in closed form by considering the form of the wavefunction in the three different regions and requiring continuity of the wavefunction and its derivative at both interfaces. The results are summarized in appendix A, where the transmission probability is given.

Qualitatively, the transmission probability is highest for electrons traveling perpendicular to the barrier and falls off rapidly as the component of $k$ parallel to the interface increases. One can understand this result in two ways. Classically, one can imagine a beam of particles that decays at a certain rate as it propagates through a barrier region. Therefore, the transmission probability for an electron with wavevector component parallel to the layers the decay will be faster, since the wavefunction will be proportional to $\exp(-\kappa z)$, where $\kappa^2$ will be given by $\kappa^2 = (2m/\hbar^2)(V - E) + k_z^2$. The quantum mechanical picture is that the oscillations of the wavefunction in the plane of the barrier due to the $k_z$ component of the wavevector represent an energy $(\hbar^2k_z^2/2m)$ associated with lateral motion of the electron. This energy is not available for getting through the barrier. Thus the expression for $\kappa^2$ can be written as $\kappa^2 = (2m/\hbar^2)(V - E')$, where $E' = E - \hbar^2k_z^2/2m$. We shall see that oscillations of the wavefunction in the plane of the barrier tend to increase the rate of decay of the wavefunction in the barrier [21].

2.5. Evanescent states

Let us next consider a more realistic picture of the barrier. In reality, the barrier will be an insulating material made up of atoms. We usually consider an insulator to be a material with no electronic states within an interval in energy (the energy gap) around the Fermi energy. Figure 3 shows the band structure of MgO for the (100)-direction. The meaning of the energy bands is that they give the energy of the propagating Bloch states as a function of the quasi-momentum, $\mathbf{k}$ where $\mathbf{k}$, describes how the wavefunction in one cell is related to the wavefunction in a neighboring cell. If the system is periodic, one can show that the wavefunction (solution to the Schödinger equation) at point $\mathbf{r}$ in one cell is proportional to the wavefunction at the corresponding point $\mathbf{r} + \mathbf{a}$ in an adjacent cell, $\psi_n(\mathbf{r} + \mathbf{a}) = c\psi_n(\mathbf{r})$ where $\mathbf{a}$ is a lattice vector. A simple argument supporting this claim is given in appendix B. The constant of proportionality, $c$ can be any complex number. However, if the wavefunction is to be normalized over a system of infinite extent, $c^*c$ must be unity, otherwise the wavefunction will diverge either for $\mathbf{r} + n\mathbf{a}$ or $\mathbf{r} - n\mathbf{a}$ as $n \rightarrow \infty$. States of this type, which can be normalized over a solid of infinite extent, are the propagating Bloch states. The Bloch condition for propagating states can be written as $\psi_n(\mathbf{r} + \mathbf{a}) = \exp(i\mathbf{k} \cdot \mathbf{a})\psi_n(\mathbf{r})$, where the vector $\mathbf{k}$ is called the wavevector. The Bloch condition, simply describes the most general way that wavefunctions on neighboring sites can }
differ by a phase. It also allows us to make a connection with the free electron model for which the wavefunction can be written as, \( \psi_k(r) = V^{-1/2} \exp(ik \cdot r) \), where the pre-factor of the square root of volume is needed so that the wavefunction will be normalized to unity over the volume \( V \).

In addition to the solutions to the Schrödinger equation that differ by a phase from one lattice constant to the next there will be solutions that differ by a factor with absolute value different from unity. Such wavefunctions are not allowed solutions if the system is infinite, because they will diverge in one direction or the other and therefore cannot be normalized. However, they are allowed if the system is finite. In fact, they are usually necessary to ensure that the wavefunction and its derivative are continuous at the boundaries between the barrier and the electrodes. These states are called evanescent states because they vanish away from the boundaries. Both the propagating states and the evanescent states come in pairs. For every propagating Bloch state describing an electron moving in the \( +z \)-direction, there will be a corresponding state with the same energy describing an electron moving in the \( -z \)-direction. Similarly every evanescent state that decays in the \( +z \)-direction will have a partner decaying in the \( -z \)-direction.

To relate, the simple barrier model to the more realistic band model for MgO, one traditionally assumes that the tunneling current occurs through virtual transitions from the Fermi energy of the electrodes to the conduction band of the MgO. The dispersion relation for this model would be given by

\[
E = E_c + \left( \frac{\hbar^2}{2m_e} \right) k_z^2 - k_\parallel^2.
\]

The corresponding wavefunction is \( \psi_k(r) = V^{-1/2} \exp(ik \cdot r) \) which we write as \( \psi_k(r) = V^{-1/2} \exp(ik_\parallel \cdot \rho + ik_z z) \). This wavefunction and dispersion relation would be valid for \( E > E_c \). For \( E < E_c \), relevant to tunneling, \( k_z^2 \), is negative so we write, \( \psi_k(r) = V^{-1/2} \exp(ik_\parallel \cdot \rho \pm ik_z z) \) where \( k_z = \left[ \frac{2m_e}{\hbar^2} (E_c - E) + k_\parallel^2 \right]^{1/2} \).

One obvious difference between the simple barrier model and MgO (or any other insulator) is that the insulator has...
valence bands as well as a conduction band. Electrons can also tunnel through the barrier via the valence bands; this would be described as ‘hole’ tunneling because it would describe a process in which a valence electron makes an upward transition from the top of the valence band to the Fermi energy of the right electrode simultaneously with the transition of an electron at the Fermi energy of the left electrode making a downward transition that fills the hole. The situation is even more interesting, because as we shall show, the red valence band (labeled $\Delta_1$) is really the same band as the red conduction band (also labeled $\Delta_1$).

The first-principles based layer KKR approach was used to calculate $k_z$ as a function of $E$ as shown in figure 4. Just as for the simple barrier model, energies exist for which no states with real $k_z(E, k_z)$ exist. However, for these energies, states exist which are imaginary or complex. In fact all of the propagating Bloch states continue as evanescent states when they are no longer valid propagating states. In particular, for MgO, the valence band with $\Delta_1$ symmetry continues through the gap region as an evanescent state for which $k_z$ is imaginary and re-emerges at the top of the gap as the conduction band. An excellent approximation for this $\Delta_1$ state in the vicinity of the gap is

$$
\frac{1}{k_z^2} = \frac{-\hbar^2}{2m_v^*(E - E_v)} + \frac{\hbar^2}{2m_c^*(E - E_c)},
$$

where $E_v$ and $m_v^*$ represent the energy and effective mass at the top of the valence band while $E_c$ and $m_c^*$ represent the analogous quantities at the bottom of the conduction band. For MgO, $m_v^*$ and $m_c^*$ seem to be the same so that the interpolation formula for the evanescent band in the gap can be simplified to

$$
\frac{\hbar^2 k_z^2}{2m^*} = \frac{(E - E_v)(E - E_c)}{(E_c - E_v)}. 
$$

The minimum value of $k_z^2$ is $[k_z^2]_{\text{min}} = -\frac{m^*(E - E_v)}{\hbar^2}$ and occurs at mid-gap, $E = (E_v + E_c)/2$. For comparison, the simple barrier model would give $k_z^2 = -\frac{m_e(E - E_c)}{\hbar^2}$ at mid-gap.

The continuation of the bands into the gap region as evanescent states can be understood on very elementary terms for MgO. A minimal model for the electronic structure in the vicinity of the gap would include the Oxygen p-states and the Mg-s state. The tight-binding Hamiltonian matrix for $k_x = 0$ and $k_y = 0$, can be written as

$$
H(k_z) = \begin{pmatrix}
E_v & w[\exp(-ik_za/2) - \exp(ik_za/2)] \\
\exp(-ik_za/2) & E_c
\end{pmatrix},
$$

where $w$ represents the interaction between the Mg-s and nearest neighbor p-states. The diagonal elements of the matrix represent the atomic energies of the Mg-s and oxygen-p states (possibly modified by terms independent of $k_z$). The off diagonal matrix elements represent interactions between the Mg-s and nearest neighbor p-states.
Figure 13. Calculated transmission probability for majority electrons for parallel alignment of the Fe electrodes for three thicknesses of the MgO barrier. The thicknesses are (top to bottom) four, eight and 12 atomic MgO layers.

The important point to notice is that the valence band and conduction bands are really the same band, connected by an evanescent state. The empirical result that

\[ \frac{\hbar^2 k_z^2}{2m^*} = \frac{(E - E_v)(E - E_c)}{(E_c - E_v)} \]

is reproduced by the two-orbital approximation if

\[ E_c = E_s, \quad E_v = E_p \quad \text{and} \quad m^* = \frac{2\hbar^2(E_c - E_v)}{a^2w^2}. \]

2.6. MgO as a symmetry filter

Returning to figure 4, one can see that the evanescent states at the Fermi energy will decay at very different rates. The \( \Delta_1 \) states will decay most slowly, the \( \Delta_5 \) states will decay much faster and the \( \Delta_2^* \) states will decay faster still. The \( \Delta_2 \) state (not shown) decays even faster. The symbols, \( \Delta_1, \Delta_5, \Delta_2, \)
Figure 14. Minority conductance for parallel alignment of the magnetic moments in the Fe electrodes. The left-hand panels show the transmission probability plotted as the vertical axis as a function of $k_x$ and $k_y$. The panels on the right show the same data in a contour plot. Brighter areas have higher conductance.

$\Delta_2$, etc. label wavefunction symmetries compatible with the square symmetry of the two-dimensional lattice of bcc Fe or rock salt structure MgO when viewed along the 001-direction. These symmetries are depicted in figure 8.

$\Delta_1$ symmetry is that of a circle. Atomic orbitals compatible with this symmetry include $s$, $p_z$, and $d_{z^2-r^2}$. $\Delta_3$ symmetry alternates in sign in either the $x$- or $y$-directions. For this reason $\Delta_3$ states are always doubly degenerate. Atomic orbitals compatible with $\Delta_3$ symmetry are $p_x$ and $p_y$ and $d_{xz}$ and $d_{yz}$. States with $\Delta_2$ and $\Delta_2'$ symmetry have more in-plane sign changes than $\Delta_1$ or $\Delta_5$. $\Delta_2$ and $\Delta_2'$ symmetries are not compatible with atomic $s$- or $p$-orbitals. Note that there is a qualitative correlation between the rate of decay of the evanescent states in MgO and the number of in-plane oscillations of the wavefunction.

Figure 4 shows that MgO can act as a symmetry filter. Incident wavefunctions of different symmetries will decay at different rates within an MgO barrier if it is epitaxial on an electrode and the two-dimensional symmetry is maintained at the interface. In particular, incident states with $\Delta_1$ symmetry should be transmitted with much higher probability than other symmetries. One way to convert this symmetry filter into a spin filter, is to find materials compatible with MgO that have propagating Bloch states with $\Delta_1$ symmetry at the Fermi energy for one spin channel but not for the other.

2.7. $\Delta_1$ Bloch states in Fe

Figure 9 shows the majority and minority bands in the (001)-direction for Fe. The Fermi energy at approximately 5 eV intersects the $\Delta_1$, $\Delta_3$ and $\Delta_2'$ bands for the majority channel, and the $\Delta_2$, $\Delta_5$ and $\Delta_2'$ bands for the minority spin channel. The up- and down-spin bands are very similar for the two spin channels. The primary difference is a downward shift of the
d-bands in the majority relative to the minority. Thus Fe is a possible system to use with MgO to take advantage of its symmetry filtering effect to make a spin-filter.

The reason that the $\Delta_1$ band is present at the Fermi energy in the majority, but not in the minority is the $\Delta_1$ gap that separates a lower $\Delta_1$ band from a higher $\Delta_1$ band for both spin-channels. Before discussing the spin-filtering effect of Fe–MgO tunnel junctions, it may be helpful to consider the origin of this $\Delta_1$ gap. As mentioned previously, $\Delta_1$ states are compatible with atomic orbitals with angular symmetries, $s$, $p_z$ and $d_{3z^2-r^2}$. In most of the ferromagnetic transition metals, the $p$-states are significantly higher in energy than the $s$ and $d$-states. Therefore, a minimal model for the $\Delta_1$ states will consist of the $s$ and $d_{3z^2-r^2}$ orbitals. For simplicity, we retain only nearest neighbor interactions, so that a tight-binding Hamiltonian to describe the system can be written for electrons propagating along (001) as,

$$\mathbf{H}(k_z) = \begin{pmatrix} E_s - w_s \cos(k_z a/2) & -w_{sd} \cos(k_z a/2) \\ -w_{sd} \cos(k_z a/2) & E_d - w_d \cos(k_z a/2) \end{pmatrix}.$$ 

Here $E_s$ and $E_d$ are the positions of the centers of the $s$- and d-bands. The parameter $w_s$ describes the interaction between s-orbitals on nearest neighbor sites in the bcc lattice and determines the width of the $s$-band. The parameter, $w_d$, plays a similar role for the $d_{3z^2-r^2}$ sub-band. The parameter, $w_{sd}$ describes the interaction between s- and $d_{3z^2-r^2}$ orbitals on neighboring sites. The energy bands can be obtained by setting the determinant of $(E \mathbf{I} - \mathbf{H}(k_z))$ to zero and solving the simple quadratic equation for $E$ as a function of $k_z$.

$$(E - E_s + w_s \cos(k_z a/2))(E - E_d + w_d \cos(k_z a/2)) - w_{sd}^2 \cos^2(k_z a/2) = 0.$$
If \( w_{sd} \) were zero, there would be separate s and d-bands as shown by the dotted (green) lines in figure 10. The presence of the interaction \( w_{sd} \) prevents the crossing of the bands and opens a hybridization gap as shown by the solid lines. The first-principles bands are shown as the red pluses for and opens a hybridization gap as shown by the solid lines.

The secular equation can also be solved for \( k_z \) as a function of \( E \). It is interesting to do this because we want to know what will happen to \( \Delta_1 \) electrons incident at an energy where there are no propagating \( \Delta_1 \) states. In figure 11, the solution of the same secular equation as in figure 10 is plotted, but in this instance we plot \( \cos(k_z a / \pi) \) versus \( E \) versus \( k_z a / \pi \). Within the \( \Delta_1 \) gap, \( \cos(k_z a / \pi) \) and \( k_z \) become complex. In this region, the absolute value of the ratio of Bloch states on neighboring sites, \( \frac{\psi_{\Delta_1}(r)}{\psi_{\Delta_1}(r+1)} \), is plotted. The probability density will decay as the square of this ratio as an electron with \( \Delta_1 \) symmetry and an energy within the \( \Delta_1 \) gap traverses a layer.

2.8. Tunneling conductance for Fe–MgO–Fe magnetic tunnel junctions

Appendix A describes in detail how the transmission probability can be calculated in the simple barrier model. It is possible to extend this approach \([19, 21–24]\) to more realistic systems in which the incident, reflected and transmitted electrons are represented by propagating Bloch waves. The result of one such calculation is shown in figure 12 for the particular case of Bloch waves of different transverse symmetries incident from the left in an Fe electrode for \( k_z = 0 \).

For majority to majority tunneling, both electrodes have propagating Bloch states with similar symmetries, \( \Delta_1 \), \( \Delta_5 \) and \( \Delta_2 \). Each of these Bloch states will be transmitted with a probability that depends on the interfacial transmission amplitudes but primarily on the rate of decay of the wavefunction in the barrier. This rate of decay can be seen to vary dramatically with the transverse symmetry of the incident Bloch state with \( \Delta_2 \) decaying much faster than \( \Delta_5 \), which in turn decays much faster than \( \Delta_1 \). These decay rates, which can be accurately estimated from the slopes of the lines within the barrier are the same as those predicted from the imaginary wavevectors that can be read off of figures 4 and 7. The primary difference between the two upper panels describing \( G^{\uparrow\downarrow} \) and \( G^{\downarrow\uparrow} \) is the absence of \( \Delta_1 \) symmetry in the minority–minority channel. For this reason, the conductance for parallel alignment is dominated by the majority spin-channel conductance.

For anti-parallel alignment (bottom two panels) we must consider contributions to the conductance from \( G^{\uparrow\downarrow} \) (left) and \( G^{\downarrow\uparrow} \) (right). For \( G^{\uparrow\downarrow} \), there is no \( \Delta_1 \) state so the conductance will be small. For \( G^{\downarrow\uparrow} \), however, there is a \( \Delta_1 \) state in the left electrode at the Fermi energy which decays relatively slowly in the barrier. However, it does not contribute to the conductance because it cannot propagate in the minority spin channel. It can be seen that the wavefunction continues to decay exponentially in the minority Fe electrode on the right-hand side of the barrier.

The arguments of the preceding paragraphs apply rigorously only for \( k_z = 0 \), i.e. for electrons traveling perpendicular to the interfaces. Figure 13 shows the calculated transmission probability as function of \( k_z \) for the majority spin channel for parallel alignment of the electrodes. It can be seen that the transmission probability decreases as the thickness of the MgO barrier increases. It is also evident that the transmission becomes more strongly concentrated near \( k_z = 0 \).

The transmission probability for minority electrons for parallel alignment of the moments in the electrodes is shown in figure 14. The rapid decay of the \( k_z = 0 \) wavefunctions in the MgO allows other contributions to become important for our idealized case with perfect two-dimensional periodicity. The minority channel conductance is strongly influenced by surface resonance states. These cause the strong peaks seen

**Figure 16.** Absolute square of the wavefunction for \( k_z = 0 \) Bloch states as a function of atomic layer number for Co–MgO–Co magnetic tunnel junctions. The left panel is for parallel alignment of the Co moments. The right panel is for anti-parallel alignment.
the $k_x$-$k_y$ plane. Similar peaks can be seen in the calculated transmission spectrum for the anti-parallel conductance (figure 15). Because of the assumed symmetry, the majority and minority channel conductances are the same for anti-parallel alignment.

2.9. Tunneling conductance for bcc Co–MgO bcc Co and CoFe–MgO–CoFe magnetic tunnel junctions

The conductance has also been calculated [25] for bcc Co electrodes (figure 16) and for CoFe electrodes (figure 17) with MgO tunnel barriers similarly to those for Fe–MgO systems. The ordered B2 phase was assumed for CoFe. For both of these systems, there is only a single majority band in the (001)-direction at the Fermi energy. This band has $\Delta_1$ symmetry. The propagating minority Bloch states at $k_z = 0$ have $\Delta_5$ and $\Delta_2'$ symmetries. As a consequence, the $k_z = 0$ decay rates for the wavefunctions in the barrier can be described quite simply.

For parallel alignment of the electrodes, the majority wavefunction with $\Delta_1$ symmetry decays much more slowly within the MgO barrier than the minority wavefunctions which have either $\Delta_5$ or $\Delta_2'$ symmetry. Thus the conductance will be dominated by the majority spin channel. For anti-parallel alignment of the electrodes, on the other hand, majority electrons in the left electrode will enter the MgO similarly to the case of parallel alignment, but cannot propagate in the right electrode because there are no $\Delta_1$ minority states available. Similarly, the minority electrons in the left electrode with $\Delta_5$ or $\Delta_2'$ symmetries will become locally majority which means that they cannot propagate because only $\Delta_1$ majority states are available.

The description of the wavefunction decay in the barrier is essentially identical for FeCo as for bcc Co. For both of these cases, systems with perfect two-dimensional symmetry at zero temperature in the absence of spin–orbit coupling would have zero contribution to the conductance for anti-parallel alignment of the electrodes. For other values of $k_z$, of course there will be contributions to the conductance. Nevertheless, an integral over $k_z$ indicates a much larger conductance for parallel alignment than for anti-parallel. For a system with a barrier consisting of eight MgO atomic layers, the ratio of parallel to anti-parallel conductance for a perfect system in the absence of spin–orbit coupling was predicted [25] to be approximately 50 for Fe–MgO–Fe, approximately 150 for bcc Co–MgO–bcc Co, and approximately 350 for CoFe–MgO–CoFe. It should be emphasized, however, that real systems are never perfectly ordered and that spin–orbit coupling is always present.

2.10. Experimental confirmation

Because the mechanism for tunneling magnetoresistance described here is quite different from that previously observed using amorphous oxide barriers, obtaining the required structures with local two-dimensional periodicity required significant effort. It was necessary, for example, to prevent oxidation of the Fe layer at the Fe–MgO interface [26], the reason for this is that O atoms in the interfacial Fe layer significantly degrade the overlap between the $\Delta_1$ states at the Fermi energy in Fe and in the MgO. In the perfect structure, the Fe electrode terminates in a square lattice of Fe atoms, immediately above each of these Fe atoms will be an O atom in the first atomic layer of MgO. The Mg atoms will sit in the centers of the squares formed by the O atoms. This configuration allows strong overlap between the Fe $d_{3z^2-r^2}$ and the O $p_z$ states. If, however, O atoms enter the interfacial Fe layer, this strong overlap is significantly degraded and the $\Delta_1$ electrons are much less likely to enter the MgO. This is illustrated in figure 18, which shows a DFT supercell calculation calculation for Fe–MgO [27].

In 2003, TMR values of 100% at low temperature and 67% at room temperature were achieved [28] using molecular beam epitaxy (MBE). In late 2004 observations of TMR in
the range of 200% at room temperature were announced [29, 30] using both MBE grown Fe–MgO–Fe [29] and sputtered CoFe–MgO–CoFe [30]. The current record (in late 2007) seems to be 1010% at low temperature and 500% at room temperature [31]. In addition, the predicted high TMR of bcc Co–MgO–bcc Co has been confirmed [32].

The prediction and discovery of symmetry filter based TMR has had a significant impact on current and potential spintronic devices. Three important aspects of these have helped to drive their rapid commercialization: (i) the high TMR is very important for most spintronic devices; (ii) the relatively low resistance resulting from the slow decay of the Δ₁ wavefunction in the MgO is also important in many types of devices such as read sensors for hard drives and spin–torque switched magnetic random access memory; and (iii) the discovery [30] that these systems could be grown by sputtering allowed them to be readily deposited using deposition tools widely available in industrial laboratories. Growth by sputter deposition requires that the system be annealed after deposition to achieve a locally crystalline barrier and electrodes.

Presently most (if not all) new hard drives appear to utilize this technology in the magnetic field sensor used for reading the information stored on disk. These materials sets are also at present the leading candidates for a new type of magnetic random access memory that is written using the spin–torque effect.

3. Summary

In summary, a brief overview of the young, but rapidly growing field of spintronics was presented. The manner in which electrons tunnel through simple insulators was also described and the physical phenomena that cause electrons whose wavefunctions are most symmetric to be preferentially transmitted were explained. It was also explained how this symmetry filtering effect can be made into a spin filtering effect by combining a symmetry filtering barrier material with electrodes that have wavefunctions with the preferentially transmitted symmetry in one spin channel, but not in the other. The resultant large spin-filtering effect has been applied in read sensors for hard drives and may soon be applied to make a new type of non-volatile solid state magnetic memory.

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Appendix A. Simple barrier model for tunneling

In this model, which is a prototype for studies of ballistic tunneling in real materials, an incident electron (on the left) generates both a reflected wave (also on the left) and a transmitted wave (on the right). In the barrier region, which separates the two regions with propagating states, the wavefunction is evanescent. The wavefunctions on the left and right are normalized so that they each carry unit flux, thus

\[ J = -\frac{i}{2} \left( \psi^* \frac{\partial \psi}{\partial z} - \frac{\partial \psi^*}{\partial z} \psi \right) = 1 \]

for each of the three wavefunctions in the leads (omitting the prefactors \( r \) and \( t \) which are the reflection and transmission amplitudes). With this normalization the sum of the reflection probability, \( R = r^* r \), and the transmission probability, \( T = t^* t \), is unity. Thus the total outgoing flux \( R + T \) equals the incident flux, unity.

The wavevectors that enter these expressions are the \( z \)-components of the wavevectors of the electrons in the leads and in the barrier,

\[
k_1 = \sqrt{\frac{2m(E - V_1)}{\hbar^2}} - k_{1,0}^2, \quad k_0 = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} + k_{1,0}^2, \quad k_2 = \sqrt{\frac{2m(E - V_2)}{\hbar^2}} - k_{2,0}^2.
\]

They depend on both the energy, \( E \) and on the component of the wavevector parallel to the layers, \( k_1 \). By requiring that the total wavefunction in each region, join continuously and smoothly to the wavefunctions in the adjacent region, one obtains four equations (2 each for \( z = 0 \) and \( z = a \)) in four unknowns \((r, t, A \text{ and } B)\). Note that the total wavefunction in
region 1 on the left is the sum of the incident and reflected waves. The four equations in four unknowns can be solved simply for the four unknowns. In particular the transmission probability is given by,

\[ T = |t|^2 = \frac{8k_1^2k_2}{(k_1^2 + \kappa_0^2)(k_2^2 + \kappa_0^2)} \cos(2\kappa_0a) + 4k_0^2k_1k_2 - (k_1^2 - \kappa_0^2)(k_2^2 - \kappa_0^2) \]

When the barrier is thick enough that \( e^{2\kappa_0a} \gg 1 \), the expression for the transmission probability simplifies considerably,

\[ T = \frac{16k_0^2k_1k_2e^{-2\kappa_0a}}{(k_1^2 + \kappa_0^2)(k_2^2 + \kappa_0^2)} = \frac{4k_0k_1}{(k_1^2 + \kappa_0^2)} \frac{4k_0k_2}{(k_2^2 + \kappa_0^2)} e^{-2\kappa_0a} = T_1T_2 e^{-2\kappa_0a}. \]

Written in this way, it is clear that the transmission probability for the simple barrier model can be factorized into three factors, one that depends on the left interface, one that depends on the right interface and one that describes the decay of the wavefunction in the barrier. \( T_1 \) and \( T_2 \) in this formula can be interpreted as the probability that an electron incident on an infinite barrier will be transmitted as an evanescent wave. Note that this factorization is sufficient to derive a Julliere-type model in which the polarizations are defined not in terms of the electrode density of states but in terms of the densities of states for the transmission probabilities. Thus the TMR for the simple barrier model is given by,

\[ \text{TMR} = \frac{2P_1P_2}{1 - P_1P_2}, \quad \text{where} \quad P_1 = \frac{T_1^\dagger - T_1^\dagger}{T_1^\dagger + T_1^\dagger} \quad \text{and} \quad P_2 = \frac{T_2^\dagger - T_2^\dagger}{T_2^\dagger + T_2^\dagger} \quad \text{for each value of} \ k_1. \]

### Appendix B. Propagating and evanescent states in periodic systems

Consider the Schrödinger equation for a periodic system,

\[ \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(r) - E \right] \psi(r) = 0. \]

Here \( V(r) \) can be the effective potential used in a first-principles DFT calculation. With complete equivalence, because the system is periodic, we can express the Schrödinger equation relative to an adjacent lattice site,

\[ \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(r + \mathbf{a}) - E \right] \psi(r + \mathbf{a}) = 0. \]

Since the potential is (by assumption) periodic, \( V(r + \mathbf{a}) = V(r) \). Thus, \( [H(r) - E]\psi(r) = 0 \) and \( [H(r) - E]\psi(r + \mathbf{a}) = 0 \). Since \( \psi(r) \) and \( \psi(r + \mathbf{a}) \) are two solutions to the same homogeneous differential equation with the same boundary conditions, they must be equal up to a constant factor. Thus \( \psi(r + \mathbf{a}) = c \psi(r) \).

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