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# Quantum transport simulation based on an equation of motion method: An application to current-perpendicular-to-the-plane giant magnetoresistance

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A tight-binding equation of motion (EOM) method for the simulation of electronic transport in complex, and inhomogeneous systems is presented. Conductance is calculated in the linear response regime where chemical potentials can mimic electrochemical potentials. The technique is first elucidated by application to several simple systems to clarify important issues. A calculation of current-perpendicular-to-the-plane giant magnetoresistance (GMR) in a Co/Cu multilayer then follows. A 67% GMR is calculated which originates primarily from spin-dependent interface resistances. The advantages of an EOM method are that complicated geometries can be considered, and interactions such as spin-orbit effects or phonons, for example, may be included easily.

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## I. INTRODUCTION

Electronic transport in complex and inhomogeneous systems is of fundamental and technological interest in many nanoscale devices. The giant magnetoresistance (GMR), effect observed in thin film magnetic multilayers is a particularly good example of such a system—see Ref. 1 for a recent review. This effect can be observed in the current-in-the-plane (CIP) or perpendicular-to-the-plane (CPP) geometry. These devices often contain ferromagnetic transition materials such as Co, Fe, or Ni whose complicated electronic structure makes a simple free-electron description invalid. In the CPP geometry the effect is dominated by spin-dependent interface resistances which are due to the electronic structure mismatch between consecutive layers. Complex systems such as this are commonly considered in the field of spintronics; often they are composed of materials with complicated and spin dependent electronic structures, and can be small enough that quantum effects are important.

There are many techniques available for studying electronic transport in such systems. The density matrix equation, or approximate versions of it such as the Boltzmann equation can be applied with success,[2–4] albeit with some difficulty for more complex systems. Approaches based on calculating transmission coefficients can be very useful, using one electron Green's functions or transmission matrices and the Landauer-Büttiker formula for conductance.[5,6] Nonequilibrium Green's function techniques such as the Keldysh formalism[7] can also be used, however, they can be restricted to highly symmetrical geometries, and in some cases the important physics can be obscured by the mathematical complexities. Kubo formula based techniques, such as the recursive tight-binding method[8–10] can be very effective, however, the inclusion of dynamical effects may prove difficult.

In this paper we demonstrate the application of an equation of motion (EOM) method for simulating quantum transport in complex, inhomogeneous systems. EOM methods take a governing dynamical equation, for example, the Schrödinger equation, and integrate it in time numerically.[11,12] Such methods have a long history and have the advantage that complicated time-dependent interactions may be included. The method presented has connections with Green's function calculations of the transmission coefficient, but differs in some important ways. The contacts are present in this method to allow current to flow and to truncate the system in such a way that the properties of the system under investigation are not appreciably affected. The method allows the inclusion of additional interactions, for example, lattice vibrations[13] and other time-dependent phenomena simply by including additional terms and equations in the EOM. With regard to lattice vibrations, a Bose-Einstein distribution of phonon frequencies can be selected within the simulation and this can be important for many semiconductor devices—for example, when there are high frequency optical modes. A tight-binding (TB) model is used for the electronic structure as this can reproduce many complex features without prohibitive computational cost. In many cases very precise description of the electronic structure is not the major issue and in situations where it is important, such as near the band gap in a semiconductor, TB can often be a very good approximation.[14]

The paper is organized in the following way. In Sec. II the EOM method is introduced. There are important issues related to the role of contacts and numerical stability that will be discussed. In Sec. III results for simple model systems using tightly bound $s$ orbitals are presented. An interface between dissimilar materials is considered, and an interface resistance for such a system is calculated. A discussion of the method when applied to simple systems is vital in order to lay a firm foundation for this and future work based on this approach, and to make comparisons with simple theoretical calculations. There are fundamental issues that apply to many different situations that can easily be obscured by the complexity of a specific problem. The method is then applied to a calculation of CPP GMR in a Co/Cu multilayer—which is the type of system which has potential device applications. The simulation of such a device using an EOM method has many advantages, for example one can include the spin-orbit interaction and simulate spin relaxation in the presence of disorder. Dynamical effects such as spin-torque driven magnetization reversal are also a possibility. However, in this paper we present this calculation mainly to demonstrate the application of the method to a complex realistic system. A more concentrated investigation of transport in such systems will follow at a later date. Many of the techniques discussed may be applied to a variety of other wave phenomena, for example, electromagnetic waves or heat transport, but in this paper we investigate fundamental issues with application to many areas of metal and semiconductor physics.

## II. TECHNIQUE

### A. Basis of the technique

In calculating the conductance of a system one may approach the problem in two different but equivalent ways. The first is to calculate the current as a response to the application of a potential difference across the system. The second is to calculate the potential difference arising as a consequence of the current flowing through the system. In both cases the current that flows is related to the difference of electrochemical (EC) potential $\Delta\Phi$ through the conductance $G$. This work is developed corresponding to the latter picture. The injection of current through some complicated system is simulated using an EOM. If the system reaches a steady state the conductance can be determined.

The EC potential $\Phi$ is the relevant potential for electron transport in metals in the absence of magnetic fields. It consists of the electrostatic potential due to space charge $\phi$ together with the chemical potential $\mu$ due to variation of electron density:

$$\Phi(\mathbf{r}) = \phi(\mathbf{r}) - \frac{1}{e}\mu(\mathbf{r}). \tag{1}$$

The relationship between chemical potential and electron density can be quite complicated. However, in linear response deviations in the number density and chemical potential can be assumed to be small enough to allow one to use the simple linear relationship

$$\delta\mu(\mathbf{r}) = \frac{\delta n(\mathbf{r})}{g(E_F)}, \tag{2}$$

where $\delta n(\mathbf{r})$ is the deviation in electronic number density and $g(E_F)$ is the density of states (DOS). In general the local DOS should be used which can vary significantly throughout an inhomogeneous system. In a macroscopically homogeneous metal in equilibrium, currents due to density gradients must balance currents due to internal electric fields. It follows that the conductivity and the diffusion coefficient must be related through the Einstein relation[15]

$$\sigma = e^2 g(E_F) D. \tag{3}$$

Chemical potential gradients are therefore equivalent to electrostatic potential gradients in linear response—despite the fact that the former does not accelerate electrons. Therefore it is very convenient to neglect the electrostatic potential and calculate the conductance by simulating electron diffusion. If a particle current $I$ and a chemical potential difference $\Delta\mu$ is calculated between two points, then the conductance is obtained using

$$G = \frac{Ie^2}{\Delta\mu}. \tag{4}$$

In the presence of a nonequilibrium current, when there are variations of chemical potential which cannot be included in the Hamiltonian, it is necessary to introduce a sensible definition of a local chemical potential in terms of local averages of density and densities of states. After all any real physical measurement involves contacts and averaging over some region of space when defining the potential difference.

The time-dependent Schrödinger equation (TDSE) is integrated numerically to simulate the dynamics of electrons passing through the system. A TB basis set is used as the short range hopping integrals lead to nearly diagonal matrices and hence large systems may be studied easily. The TB wave function is assumed to have the following form:

$$\Psi(\mathbf{r}) = \sum_{\gamma} a_\gamma \phi_\gamma(\mathbf{r}), \tag{5}$$

where $a_\gamma$ is a complex amplitude associated with each orbital. In this abbreviated notation the suffix $\gamma$ denotes an atomic orbital on a particular site with a given spin eigenstate, given by the orbital wave function $\phi_\gamma(\mathbf{r})$. The parametrized TB electronic structure model employed has hopping matrix elements that have been used as fitting parameters to agree with more accurate band structure calculations.[16] A two-center orthogonal representation containing $s$, $p$, and $d$ orbitals is used and yields electronic structures, particularly for transition metals, that are in reasonable agreement with more numerically demanding methods. The TB TDSE that must be numerically integrated takes a particulary simple functional form

$$i\hbar\frac{\partial}{\partial t}a_\gamma(t) - a_\gamma(t)E_\gamma - \sum_{\gamma'} a_{\gamma'}(t)V_{\gamma\gamma'} = 0, \tag{6}$$

where $V_{\gamma\gamma'}$ are the hopping matrix elements between the various orbitals which in general can depend on time and $E_\gamma$ are the set of orbital energies. The actual functional form of the TDSE is simplified by the fact that many of the hopping matrix elements are zero and others posses certain symmetry properties.[17] The state of the system at any instant in time is completely specified by the set of complex amplitudes $a_\gamma(t)$.

### B. Modeling current flow

The way in which leads are attached to a system defines a conductance; this is as true for calculations as it is experimentally. In calculations of conductance the leads can also act to truncate the system under investigation; as one would hope the details of the leads far away from the system should not influence the conductance. There are some systems where the nature of the contact can have a great impact on results, molecular systems, for example,[18] and in these cases calculations must carefully consider the boundary conditions. However, for the complex, and inhomogeneous, metallic systems considered here the complexity within the device is more crucial and we present an EOM method for such systems.

It is common when using Green's function techniques to decouple the system by attaching semi-infinite disordered leads to the system. In the TB recursion method, for example, this serves two important purposes. It allows one to use the Kubo formula for the conductance such that it corresponds to a Landauer-Büttiker type transmission calculation;[19,20] the original application of the Kubo formula corresponds to a spatial average of conductance. Secondly, it ensures that the eigenstates of the system form a continuum so that the dc conductance at the Fermi energy can be defined sensibly. The effect of the leads on the system can be seen as analogous to introducing a complex self-energy to the Green's function of the isolated system.[21] In many calculations the leads are present more for technical reasons than to represent reality—after all real contacts are sometimes superconducting, especially for perpendicular to the plane measurements on small structures, and may give rise to additional effects.

In this EOM method we represent the leads by allowing a nonequilibrium current to flow between two regions in a way that does not significantly affect the properties of the system. The absorption of electrons can be included by analogy with the complex self-energy discussed above. A negative imaginary part can be added to the orbital site energies $E_\gamma$ in regions where the leads are present. One could use a TB recursive Green's function type of calculation to determine the magnitude this should have, however, as the leads are to perturb the system as weakly as possible we can simply chose the imaginary part to maximize the transmission of electrons out of the system. One can obtain some idea of how to achieve this by calculating the reflection coefficient for a simple one-dimensional chain of $s$ orbitals terminated by an imaginary site energy $-i\eta$. The orbital site energy has been chosen to be zero on all other sites for convenience. Equation (7) expresses this dependence as a function of the electrons energy $E$ expressed in units of the interatomic hopping matrix element $V$:

$$|R|^2 = \frac{1-\eta\sqrt{4-E^2}+\eta^2}{1+\eta\sqrt{4-E^2}+\eta^2}. \tag{7}$$

The minimum of this function occurs at $\eta=1$, which in the units used corresponds to $E_0=-i|V|$. Reflection is minimized when the electrons are in the center of the band. Using this as a guide in the extension to three dimensions and complex electronic structures, we find that the transmission is approximately optimized by matching the imaginary component of the orbital energy to the dominant hopping coupling mechanism for that orbital. This was found by studying the decay rate of eigenstates with energy $E$. The effect of this imaginary energy is similar to the effect of an acoustic absorber or the imaginary part of the refractive index in an optical system.

The injection of electrons into a region of the system is included by the addition of an appropriate source term to the EOM. Electrons are introduced at the Fermi energy, and subsequently diffuse through the system before being absorbed into the lead. In this way an equilibrium steady state current can be imposed on the system. The use of a source term in this way may be a familiar concept in other wave equations, but as it plays a central role in this method a more detailed discussion will follow.

If a point source of outgoing waves is present at $\mathbf{r}'$ the wave function at any other point $\mathbf{r}$ is given simply by the retarded Green's function $G(\mathbf{r},\mathbf{r}')$, which is defined in the usual way,[22]

$$(E+i\eta-H)G(\mathbf{r},\mathbf{r}')=\delta(\mathbf{r}-\mathbf{r}'), \tag{8}$$

where the small imaginary part, $i\eta$ is present to ensure causality. The calculation of the Green's function in free space is straightforward, and one can verify easily that the outgoing waves carry a net current of particles away from the point source. On Fourier transform one obtains an equation of motion which if modified with a time-harmonic term defines a Green's function for a particular energy $E'$:

$$\left(i\hbar\frac{\partial}{\partial t}-H\right)G(\mathbf{r},\mathbf{r}',t)=\delta(\mathbf{r}-\mathbf{r}')e^{-iE't/\hbar}. \tag{9}$$

An infinitesimal imaginary part should be included in $E'$ corresponding to an adiabatic switching on of the source term in order to avoid transients.

In order to model electron injection a TDSE of the following form is considered:

$$\left(i\hbar\frac{\partial}{\partial t}-H\right)\Psi(\mathbf{r},t)=f(\mathbf{r})e^{-iE't/\hbar}, \tag{10}$$

where $f(\mathbf{r})$ is nonzero in the region containing the sources. This equation can be integrated numerically in time and corresponds to the presence of sources of electrons with energy $E'$, in the region $f(\mathbf{r})$. Source, or driving terms such as this are often used to describe the introduction of particles or energy in differential equations. The diffusion equation, for example, can be used to describe the conduction of heat, and sources added to this equation correspond to heat sources. Importantly the use of source terms with the schrödinger equation has been considered,[23] and is similar to the addition of source terms to the classical wave equation, modeling sound waves, for example.[24]

Sources are present on all atoms that are adjacent to the lead. In practice these sources are switched on at $t=0$ as opposed to adiabatically, however, the transients become unimportant after a short time and are negligible in the steady state. In the TB formalism the source terms take the following form:

$$S_\gamma e^{-iE't/\hbar} \tag{11}$$

which are added to the right-hand side of Eq. (6). The square of the source magnitude $S_\gamma^2$ is directly proportional to the current supplied by the point source. Electrons are injected at the Fermi energy with a narrow spread of energies to smooth out any finite size effects due to the finite energy separation of the eigenstates.

This procedure for the injection and removal of electrons can be regarded as a simple way to set up an equilibrium steady state current through a system. A four-point conductance is calculated using this method, which is defined in terms of density differences inside the system. The precise details of the boundary conditions are not important, providing they impose a current of electrons with energy $E$ which settles down to a steady state.

This EOM technique allows one to calculate the steady state wave function in a system subject to boundary conditions that impose a net current flow between two leads. Once this is obtained the diffusion coefficient and hence the conductance can be determined. The EOM method is suited to the inclusion of additional terms in the Hamiltonian, and molecular dynamics may be used to include phonon interactions. The presence of complex energies, used to absorb electrons, makes the commonly used leap frog method for numerical integration unstable. Instead a second order Runge-Kutta technique must be used but it still allows time-steps comparable with the LF method. Many of the ideas explored here have connections with pioneering work carried out many years ago and we would cite the work on thermal conduction by Payton, Rich, and Visscher[25] as a prime example.

## III. RESULTS

### A. Anderson model disordered wire

The application of the method to a simple system is essential as it allows one to verify the precision of the calculation by a comparison to an alternative theoretical calculation. A simple cubic system of $s$ orbitals coupled to nearest neighbors only, with hopping matrix elements of $V=1$ eV is considered. Diagonal Anderson disorder is introduced to the orbital energies with a full width spread $W=2$ eV, hence well below the localization transition for three dimensions. 24 750 atoms are simulated in a $15\times15\times110$ configuration, with the current parallel to the length. Periodic boundary conditions are applied in the transverse $x$ and $y$ directions in order to minimize the effect of surface scattering, although box boundary conditions can be used if desired with little effect for large enough systems. The Fermi level is chosen in the center of the band and all energies are referenced to this as the energy zero.

Steady state is defined by the requirement that the norm of the wavefunction integrated over the whole system is constant in time. Steady state for this system is reached in about 1 ps using a time step of 5 as, hence requiring about 200 000 iterations—as shown in Fig. 1(a). Systems with higher resistances require longer to reach steady state but normally this is not a problem. The conductance of the system is calculated by examining the spatial dependence of the plane averaged chemical potential and calculating the current. The electric current density is calculated using the following expression consistent with using the TB approximation

$$\mathbf{J}=\mathrm{Re}\left(\frac{ie}{\hbar\Omega}\sum_{\gamma\gamma'}a_{\gamma}a^{*}_{\gamma}V_{\gamma\gamma'}(\mathbf{r}_{\gamma}-\mathbf{r}_{\gamma'})\right), \tag{12}$$

where $\Omega$ is the volume over which the sum is performed. There are nonequilibrium fluctuations about the steady state mean current, however for dc conductance only the time average of the current is required. In calculating the chemical potential the bulk DOS of the material is used. This is obtained using a standard Green's function technique.[26,27] We consider the variation between planes 10 and 100 to ensure we are calculating the bulk resistivity eliminating edge effects—corresponding to a four point measurement [Fig. 1(b)]. The magnitude of the chemical potential is actually irrelevant because the EOM is linear in the magnitude of the inhomogeneous source term: both the current and the potential scale as $S_{\alpha}^{2}$.

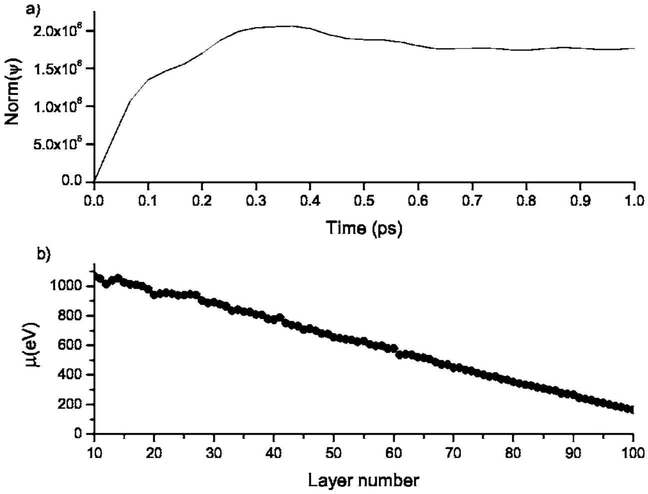

FIG. 1. Results for a simple cubic Anderson model wire with $V=1$ eV, $W=2$ eV, and lattice spacing $d=3.17$ Å. (a) The evolution of the simulation to steady state. (b) The chemical potential averaged over planes of atoms.

The calculated resistivity of this system is 126 $\mu\Omega$ cm per spin, and is not significantly changed by ensemble averaging due to the fairly large size of the system. As a comparison, we have calculated the resistivity by solving the Boltzmann equation in the relaxation time approximation. The Born approximation is used for the scattering rate—which is a reasonable approximation for this system as the resistivity scales with $W^2$ at least up to $W/V=5$. The integral over the Fermi surface is computed numerically using a Monte Carlo technique. This approximate calculation of the resistivity is only 10% larger than that calculated from the diffusion simulation.

### B. Inhomogeneous systems

As this method will eventually be applied to complex, inhomogeneous, structures where there may be additional complicating effects, it is essential to apply the method to some simpler inhomogeneous systems. We again consider a simple cubic $s$-orbital system consisting of a trilayer of varying disorder with the current perpendicular to the planes (CPP). The central layer has 50% more disorder than the outer layers and each layer is of equal thickness (Fig. 2). It is clear how the slope in chemical potential increases in the more resistive central region. The resistance of the entire system is found to be well described by the series combination of the resistances of each layer—as one might expect for the values of $W/V$ used.

In the case of real multilayers there will not only be variations in disorder, but also in electronic structure, and this will

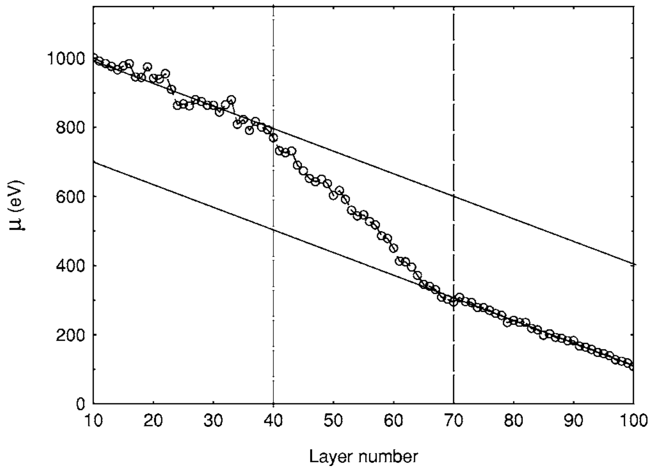

FIG. 2. The steady state chemical potential profile in a trilayer with different disorder in each layer (constant hopping matrix $V$ $=1$ eV throughout). Left to right: $W/V=2$, $W/V=3$, $W/V=2$. The solid lines are a guide to the eye.

be very important for reflection effects and interface resistances. A trilayer where the hopping matrix element is different in each of the layers is considered to explore this. This has the effect of changing the electronic structure and DOS in each of the layers. In this simple situation the resistivity only depends upon the disorder parameter $W/V$, and this is chosen to be unity throughout the system—corresponding to a bulk resistivity of 32 $\mu\Omega$ cm per spin in all layers. At the interface between two materials the average of the hopping matrix elements is used. In this situation it is observed that the electron number density in a given layer reflects the bulk DOS in that layer [Fig. 3(a)], namely, more electrons are needed in certain regions to ensure a uniform drop in chemical potential across the system. Similar behavior will be shown in simulations of magnetic multilayers. However if the mismatch in electronic structure across an interface is significant, the reflection coefficient will lead to an additional interface resistance manifested by a discontinuous drop in chemical potential.

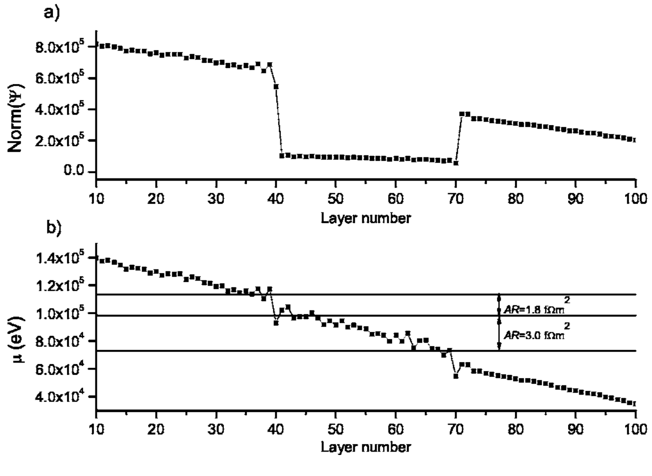

FIG. 3. Results for a trilayer of materials with the same value for the disorder parameter $W/V=1$, but with different hopping matrix elements $V$ in each layer. Left to right: $V=0.5$, 3, 0.5 eV. (a) The norm of the wave function in each plane. (b) The chemical potential profile.

The transformation between electron number density and chemical potential is obtained using the bulk DOS in a layer. Care must be taken with the identification of discontinuities in chemical potential at interfaces as boundary resistances; there is a subtle interplay of diffusive and interface effects.[28,29] Mindful of these considerations the chemical potential profile of the trilayer structure is shown in Fig. 3(b) The gradient of chemical potential in each layer is equal, demonstrating graphically that each layer has the same bulk resistivity. It is evident there is an effect of the interface, however, it would not be wise to evaluate numerically the resistance-area product from the data. If the potential either side of the device is measured within contacts with a well-defined DOS, then the calculated resistivity will include any interface resistances despite difficulty in some situations with separating the bulk and interface contributions—however, this is the reality.

An average transmission coefficient of about 80% has been calculated using a recursive Green's function method for an interface with no disorder. Following rarely cited work by Little,[30] and related works by Landauer[28] and Buttiker,[6] we have solved the Boltzmann equation to give an expression for the resistance-area product of an interface

$$\mathrm{AR}=8\frac{\pi^3}{e^2}\frac{\left(1-\dfrac{\overline{|v_{L(R)}(\mathbf{k})|^2\tau_{L(R)}(\mathbf{k})T_{\leftrightarrow}(\mathbf{k})}}{\overline{|v_{L(R)}(\mathbf{k})|^2\tau_{L(R)}(\mathbf{k})}}\right)}{\overline{|v_{L(R)}(\mathbf{k})|T_{\leftrightarrow}(\mathbf{k})}}. \qquad (13)$$

This expression assumes the current is flowing parallel to one of the crystal axes and normal to an ideal interface between materials labeled by $L$ and $R$. For each side of the interface the component of group velocity normal to the interface $v(\mathbf{k})$ and the Boltzmann relaxation time $\tau(\mathbf{k})$ is given by the appropriate suffix. The bars over the terms indicate the average over the Fermi surfaces of both materials either side of the interface. The transmission coefficient $T_{\leftrightarrow}(\mathbf{k})$ is the transmission coefficient from $L$ to $R$ if averaging over Fermi surface $L$ or from $R$ to $L$ if averaging over Fermi surface $R$. If simple approximations are used Eq. (13) reduces to the four-point Landauer formula as it should. This calculation predicts each interface in this trilayer contributes a resistance area product $\mathrm{AR}=1.8\ \mathrm{f}\Omega\, m^2$, compared to the bulk resistance for each layer $\mathrm{AR}=3.0\ \mathrm{f}\Omega\, m^2$, which is determined by the ratio $W/V$. The chemical potential drops associated with these values are indicated by the horizontal lines in Fig. 3(b), and they seem consistent with the data. In the case of realistic band structures with $s$, $p$, and $d$ orbitals, the interface resistance is likely to be significant as the Fermi surfaces are complex with large differences on each side.

### C. CPP Giant magnetoresistance

We now turn to the main focus of this work CPP GMR, which has been the subject of numerous experimental and theoretical investigations. The CPP geometry lends itself to a straightforward interpretation of the effect in terms of spin-dependent transmission through the inhomogeneous struc-

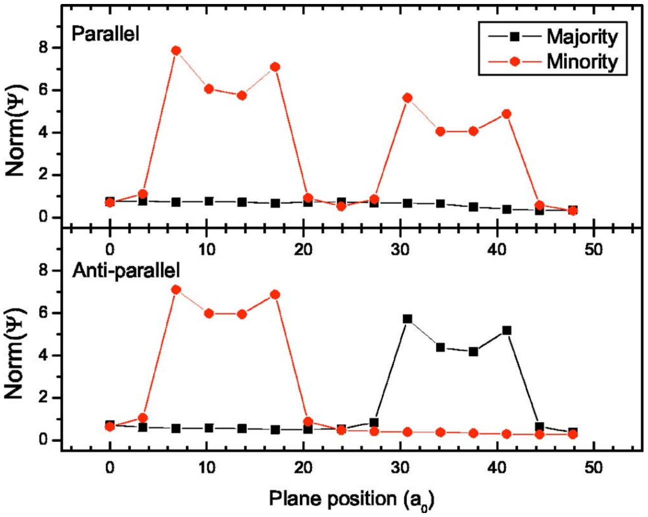

FIG. 4. (Color online.) The steady-state, norm of the wave function in each plane for parallel (P) and anti-parallel (AP) configurations ($a_0$=0.529 Å).

ture. Often simple two-current series resistor models can be used to explain the effect in terms spin-dependent interface, and bulk resistances. However, in some cases the mean-free path can be significantly large leading to proximity effects.[31] The spin-diffusion length $l_{sf}$ can also be an important scaling length for the GMR effect. It is defined as the length-scale over which a spin imbalanced chemical potential decays, and is therefore related to the spin-relaxation time and the resistivity.[3]

As an important demonstration of the EOM method we calculate the CPP GMR in a multilayer containing Co and Cu. The electronic structure is modeled with a $s$, $p$, and $d$ orbital TB parametrization.[16] It has been fitted to self-consistent augmented plane wave calculations[32] such that the Co electronic structure is appropriately spin-polarized. A $Co_4Cu_3Co_4$ trilayer is considered (subscripts denote monolayers), with fcc crystal structure and the 001 direction perpendicular to the planes. The lattice constant of both Co and Cu is taken to be 3.61 Å. Across the interfaces an average of hopping matrix elements is taken as in Sec. III B. Diagonal Anderson disorder is included with a full width of 0.5 eV in order to give realistic bulk resistances for Cu and Co.[33] Additional Cu planes are added on either side of the structure to serve as contacts in which the conductance can be defined; they enable a definition of chemical potential difference across the device in terms of the DOS of the Cu only. The spin relaxation length for this system can be estimated to be at least 100 nm, which is considerably larger than the 3 nm length of the system. This result was obtained from EOM simulations of spin relaxation, and a comprehensive discussion of such calculations will follow at a later date. As spin relaxation is negligible for this system it will not be included in this calculation, and this is consistent with experimental evidence.[34]

Figure 4 shows the steady-state norm of the wave function in each plane for parallel (P) and anti-parallel (AP) configurations. The AR for minority spins in the P configuration is 3.0 f$\Omega$ $m^2$, while for the well matched majority spins it is 0.7 f$\Omega$ $m^2$. In the AP configuration both spins have AR =2.0 f$\Omega$ $m^2$. This leads to a 67% GMR, defined in the usual way, and this value compares well with other theoretical calculations.[10] There are peaks in electron density near Co/Cu interfaces, and these are due to a combination of two effects. There is a depression of the local DOS in the minority Co adjacent to the Cu. This means the number density must decrease to reflect the chemical potential correctly. There is also electron accumulation due to the reflection at the interface. It would not be meaningful to extract the interface resistances, but it is clear that the total resistance is dominated by them. If one considers copper, with a resistivity of 7.2 $\mu\Omega$ cm per spin and of the same length as the multilayer, it would have a resistance-area product of only 0.2 f$\Omega$ $m^2$.

## IV. SUMMARY

An EOM method that may be applied to simulate a wide range of devices has been presented. The technique is suited to the inclusion of complex and dynamical effects, without the need for excessive computing resources. Within the linear response approximation, the method is well suited to modeling macroscopically inhomogeneous systems, such as magnetic multilayers. One may also consider complicated geometries, for example CIP GMR, which can prove difficult to incorporate into alternative methods. The calculation of a potential in response to an applied current has the advantage that assumptions about boundary conditions on the potential need not be made. As a demonstration of the method to a complex and realistic device, a 67% CPP GMR was calculated for a Co/Cu multilayer, which was found to be caused primarily by spin-dependent interface resistances.

The extension of this method to include the spin-orbit interaction as a mechanism for spin-relaxation is straightforward but we will present this work elsewhere as there are interesting additional issues to be described. Another aspect of this method for future development is the potential to calculate self-consistent electrostatic potentials, using Coulomb's law or Poisson's equation for example. Calculations which do not involve consideration of space charge are common, but in many semiconductor device calculations using the Boltzmann equation the space charge plays a central role—field effect transistor simulations, for example. This extension, beyond linear response, is not trivial as there is need to find a way of incorporating the Pauli principle into the calculations. However the ability to consider such things within this formalism is an important advantage of a quantum EOM method.

## ACKNOWLEDGMENTS

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[1] E. Y. Tsymbal and D. G. Pettifor, *Solid State Physics* (Academic Press, San Diego, 2001), Vol. 56, pp. 113–237.

[2] F. Warkusz, Prog. Surf. Sci. **10**, 287 (1980).

[3] T. Valet and A. Fert, Phys. Rev. B **48**, 7099 (1993).

[4] M. D. Stiles and D. R. Penn, Phys. Rev. B **61**, 3200 (2000).

[5] R. Landauer, IBM J. Res. Dev. **1**, 223 (1957).

[6] M. Büttiker, Y. Imry, R. Landauer, and S. Pinhas, Phys. Rev. B **31**, 6207 (1985).

[7] C. Heide, R. J. Elliott, and N. S. Wingreen, Phys. Rev. B **59**, 4287 (1999).

[8] P. A. Lee and D. S. Fisher, Phys. Rev. Lett. **47**, 882 (1981).

[9] J. Mathon, A. Umerski, and M. Villeret, Phys. Rev. B **55**, 14 378 (1997).

[10] E. Y. Tsymbal, Phys. Rev. B **62**, R3608 (2000).

[11] B. Kramer and D. Weaire, J. Phys. C **11**, L5 (1978).

[12] P. Prelovsek, Solid State Commun. **31**, 179 (1979).

[13] J. Carter, L. A. Michez, B. J. Hickey, and G. J. Morgan, Modell. Simul. Mater. Sci. Eng. **9**, 37 (2000).

[14] N. Bernstein, M. J. Mehl, and D. A. Papaconstantopoulos, Phys. Rev. B **66**, 075212 (2002).

[15] P. Butcher, J. Phys. C **5**, 3164 (1972).

[16] D. A. Papaconstantopolous, *Handbook of the Bandstructure of Elemental Solids* (Plenum Press, New York, 1986).

[17] J. C. Slater and G. F. Koster, Phys. Rev. **94**, 1498 (1954).

[18] K. W. Hipps, Science **294**, 536 (2001).

[19] D. C. Langreth and E. Abrahams, Phys. Rev. B **24**, 2978 (1981).

[20] B. K. Nikolić, Phys. Rev. B **64**, 165303 (2001).

[21] S. Datta, *Electronic Transport in Mesoscopic Systems* (Cambridge University Press, Cambridge, 1995).

[22] G. Rickayzen, *Green's Functions and Condensed Matter* (Academic Press, London, 1980).

[23] H. Tanaka, Phys. Rev. B **57**, 2168 (1998).

[24] P. A. Martin, SIAM J. Appl. Math. **64**, 297 (2003).

[25] D. N. Payton, M. Rich, and W. M. Visscher, Phys. Rev. **160**, 706 (1967).

[26] R. Alben, M. Blume, H. Krakauer, and L. Schwartz, Phys. Rev. B **12**, 4090 (1975).

[27] B. Kramer, A. MacKinnon, and D. Weaire, J. Phys. F: Met. Phys. **11**, 1833 (1981).

[28] R. Landauer, Phys. Rev. B **52**, 11 225 (1995).

[29] S. Zhang and P. M. Levy, Phys. Rev. B **57**, 5336 (1998).

[30] W. A. Little, Can. J. Phys. **37**, 334 (1959).

[31] R. J. Baxter, D. G. Pettifor, and E. Y. Tsymbal, Phys. Rev. B **71**, 024415 (2005).

[32] J. R. Anderson, D. A. Papaconstantopoulos, L. L. Boyer, and J. E. Schirber, Phys. Rev. B **20**, 3172 (1979).

[33] E. Y. Tsymbal and D. G. Pettifor, Phys. Rev. B **54**, 15 314 (1996).

[34] F. J. Jedema, A. T. Filip, and B. J. van Wees, Nature (London) **410**, 345 (2001).