Interfacial scattering in magnetic multilayers and spin valves

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We consider electron transport in magnetic multilayers. In particular, we consider how electron transport is affected by disorder at the interface between two layers. Standard semiclassical approaches characterize diffusive scattering at interfaces with a specularity constant S such that S is the fraction of electrons that are specularly scattered. S is typically considered to be the same for the reflected and transmitted electron beams. Here we show for two models of interfacial disorder that (a) S is not a constant, but depends on the angle of incidence as well as the energy and the degree of interfacial disorder, and (b) S is different for reflected and transmitted electrons. The two different models that we consider are (1) random point scatterers at a planar interface between layers in a free electron approximation and (2) random substitutional disorder of atoms on atomic layers near the interface. The latter model is treated within the coherent potential approximation using the layer Korringa-Kohn-Rostoker method. The fraction of electrons scattered diffusely $[1-S(\mathbf{k}_{\|})]$ is shown to have the same dependence on $\mathbf{k}_{\|}$ (i.e., angle of incidence) in the free electron limit of model (2) as in model (1). Model (2) provides a realistic description of interfacial scattering that can be readily evaluated for technologically important systems such as Co-Cu.

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I. INTRODUCTION

The discovery of giant magnetoresistance[1] (GMR) and the reemergence of tunneling magnetoresistance research[2–4] have led to active study of electronic transport in layered magnetic systems. Magnetoresistance in these systems results both from spin-dependent scattering of the electrons within the layer and from spin-dependent scattering at the interfaces. Information on the scattering within the layers can be obtained experimentally by measuring the sheet resistance of individual films as a function of thickness. This allows one to infer effective electron lifetimes for the nonmagnetic layers and to obtain constraints on the lifetimes in the two spin channels for the magnetic layers. Information on electron scattering rates at interfaces is more difficult to obtain.

Advances in both molecular dynamics simulations and experimental techniques are now providing crucial information on the makeup of multilayer interface regions.[5,6] These studies present convincing evidence that the interfaces in some technologically important multilayers can be approximated as locally crystalline with interdiffusion of different atom species occurring within a few layers of the interface. We will adopt this model for the interfacial structure and investigate the effects of disorder on the specular transmission and reflection and on the diffuse scattering.

While several studies have attempted to incorporate diffusive scattering into semiclassical and quantum interface models, most have relied on approximations in which the probability for diffuse scattering was assumed to be independent of the angle of incidence of the electron and of whether the electron was reflected or transmitted.[7,8] This approach is similar to the method used by Fuchs over 60 years ago to model conductivity in thin metallic films.[9,10] In order to satisfy boundary conditions for the Boltzmann transport equation, Fuchs assumed that each electron incident on a surface had a probability P of being specularly reflected and a probability $(1-P)$ of being diffusely (and isotropically) reflected (Fig. 1). The specular reflection probability P was assumed to be the same for all electrons, independent of the angle of incidence. A similar approach that invoked a constant specular transmission and reflection probability S for electrons incident on interfaces was introduced by Hood and Falicov[7] and has been used in other semiclassical models for multilayer transport.[8,11] A number of papers have addressed these issues for free electron scattering at surfaces. Expressions have been developed which incorporate an angular dependence of the S parameter for the case of reflection from rough exterior surfaces.[12,13]

The importance of specular scattering has been emphasized by recent experimental studies that have used oxide layers to enhance specular scattering and increase the giant

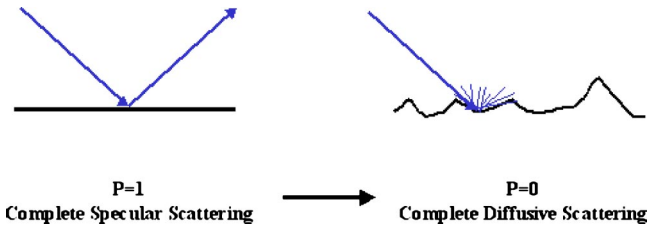

FIG. 1. (Color online) The specularity parameter P is used for matching boundary conditions in the semiclassical Boltzmann transport equation. The dependence of the specularity parameter on roughness is shown for two extremes cases: a smooth interface ($P=1$) and a rough interface ($P=0$).

magnetoresistance effect in spin valves and magnetic multilayers.[16] While these techniques have been successful in raising GMR, a detailed theory of the relationship between interfacial structure and specular scattering that can be applied to real materials remains elusive. It should be noted that a novel approach to the problem of scattering at disordered interfaces which utilizes random matrix theory has been presented recently.[17,18] In addition, the conductance through magnetic multilayers with simulated disorder using relatively small supercells has also been calculated.[19]

A clear understanding of the probability for specular scattering at interfaces is essential for the success of both quantum[20] and semiclassical[8] transport models. It is also expected to be extremely important in understanding spin-dependent tunneling experiments. Recent calculations[21–23] have predicted extremely large tunneling magnetoresistance for certain systems based on the assumption of transverse momentum conserving (i.e., specular) transmission through interfaces. A better understanding of how these predictions are affected by interfacial disorder is badly needed.

In this paper, we investigate two models for scattering at an interface between layers. We first examine interfacial scattering within a free electron model with a steplike interface in which random point scatterers are confined to the interfacial plane. We also consider a more realistic model in which Bloch electrons encounter an interface between cobalt and copper in which there is interdiffusion between the cobalt and copper atoms over one or more atomic layers at the interface. In this model the electronic structure is calculated from first principles using the layer Korringa-Kohn-Rostoker (LKKR) technique[24] with the disorder being treated within the coherent potential approximation (CPA).[25–27] We show that both models lead to an S parameter that depends on $\mathbf{k}_\parallel$.

The paper is organized into the following sections. In Sec. II, the specular and diffuse scattering of free electrons from random point scatterers confined to an interface is calculated to lowest nonvanishing order in the strength of the potentials using a Green-function-based technique. Closed-form expressions are obtained for the specularity parameters for transmission and reflection. In Sec. III, we compare results from the LKKR-CPA approach with the Green's function technique for the case of free electrons. We also determine the specularity parameter for a Co|Cu interface. Finally, in Sec. IV, we discuss some of the implications of this research on current Boltzmann transport models.

II. SPECULAR AND DIFFUSE SCATTERING FOR THE FREE ELECTRON MODEL

Consider an interface between two perfectly periodic layers. A Bloch electron incident from one layer will be either reflected back into that layer or transmitted through the interface to the opposite layer. If there is two-dimensional periodicity in the plane of the layers including the interfacial region, then the component of the crystal momentum of the electrons parallel to the layers, $\mathbf{k}_\parallel$, will be conserved and the Bloch electron will be reflected with amplitude $r(\mathbf{k}_\parallel)$ and transmitted with amplitude $t(\mathbf{k}_\parallel)$. If, however, the interface is disordered, $\mathbf{k}_\parallel$ may no longer be conserved. In this section we shall investigate these effects for the model of free electrons with random point scatterers (FERPS).[13]

Let $G_0^{+(-)}(\mathbf{r},\mathbf{r}';E)$ be the retarded (advanced) one electron Green function for a system with a single interface at $z=0$. The electron is assumed to move in a homogeneous potential U_1 for $z<0$ and U_2 for $z>0$. The Green function satisfies the equation

$$\left[E+\frac{\hbar^2}{2m}\nabla^2-U(z)\right]\mathbf{G}_0^+(\mathbf{r},\mathbf{r}';E)=\delta(\mathbf{r}-\mathbf{r}'). \tag{1}$$

Here, the energy is assumed to have an infinitesimal positive imaginary part. The advanced Green function satisfies the same equation, but with the energy having an infinitesimal negative imaginary part. Following standard techniques, we take advantage of the two-dimensional homogeneity of the system in the absence of impurities to write the Green function as

$$\mathbf{G}_0^+(\mathbf{r},\mathbf{r}';E)=\frac{1}{4\pi^2}\int d\mathbf{k}_\parallel e^{i\mathbf{k}_\parallel\cdot\rho}G_0^+(z,z';E,\mathbf{k}_\parallel), \tag{2}$$

where $\boldsymbol{\rho}$ is a two-dimensional vector in the plane of the interface, $\boldsymbol{\rho}=(x-x')\hat{x}+(y-y')\hat{y}$. By writing

$$\delta(\mathbf{r}-\mathbf{r}')=\frac{\delta(z-z')}{4\pi^2}\int d\mathbf{k}_\parallel e^{i\mathbf{k}_\parallel\cdot\rho}, \tag{3}$$

we obtain immediately the equation for the one-dimensional Green function $G_0^+(z,z';E,\mathbf{k}_\parallel)$:

$$\left(\frac{d^2}{dz^2}+\frac{2m}{\hbar^2}[E-U(z)]-k_\parallel^2\right)G_0^+(z,z';E,\mathbf{k}_\parallel)$$

$$=\frac{2m}{\hbar^2}\delta(z-z'). \tag{4}$$

This equation has a solution of the form

$$G(z,z';E,\mathbf{k}_\parallel)=\frac{2m}{\hbar^2}\frac{\Psi_L(z_<)\Psi_R(z_>)}{W}, \tag{5}$$

where $\Psi_L(z)$ and $\Psi_R(z)$ are solutions to the homogeneous Schrödinger equation, satisfying boundary conditions on the left and right sides, respectively. For the retarded Green function, Ψ_R vanishes for $z\rightarrow+\infty$ and Ψ_L vanishes for $z\rightarrow-\infty$. W represents the Wronskian of the two solutions,

$$W=\Psi_L(z)\frac{d\Psi_R(z)}{dz}-\frac{d\Psi_L(z)}{dz}\Psi_R(z), \tag{6}$$

which can easily be shown to be independent of z.

Writing $\Psi_L(\mathbf{r})$ and $\Psi_R(\mathbf{r})$ as

$$\Psi_L(z)=e^{-ik_2z}+r_Le^{ik_2z}, \quad z>0,$$

$$\Psi_L(z)=t_Le^{-ik_1z}, \quad z<0,$$

$$\Psi_R(z)=t_Re^{ik_2z}, \quad z>0,$$

$$\Psi_R(z)=e^{ik_1z}+r_Re^{-ik_1z}, \quad z<0, \tag{7}$$

we obtain $G^+(z,z';E,\mathbf{k}_\parallel)$ for the particular case of a single interface at $z=0$. The advanced Green function would have been constructed from wave functions having opposite signs for the exponentials. Defining the z component of the momentum on either side of the interface as $k_1=\sqrt{(2m/\hbar^2)(E-U_1)-k_\parallel^2}$ and $k_2=\sqrt{(2m/\hbar^2)(E-U_2)-k_\parallel^2}$ and suppressing the arguments E and $\mathbf{k}_\parallel$, we write the Green function as

$$G_0^+(z,z')=\frac{2m}{\hbar^2}\frac{t_R}{2ik_1}e^{-ik_1z}e^{ik_2z'}, \quad z<0, \quad z'>0,$$

$$G_0^+(z,z')=\frac{2m}{\hbar^2}\frac{t_L}{2ik_2}e^{-ik_1z'}e^{ik_2z}, \quad z>0, \quad z'<0,$$

$$G_0^+(z,z')=\frac{2m}{\hbar^2}\frac{1}{2ik_1}[e^{ik_1|z-z'|}+r_Re^{-ik_1(z+z')}], \quad z<0, \quad z'<0,$$

$$G_0^+(z,z')=\frac{2m}{\hbar^2}\frac{1}{2ik_2}[e^{ik_2|z-z'|}+r_Le^{-ik_2(z+z')}], \quad z>0, \quad z'>0. \tag{8}$$

Here t_L, t_R, r_L, and r_R are determined by boundary conditions at the interface. These quantities and the Wronskian of the system can be expressed in terms of k_1 and k_2:

$$t_L=\frac{2k_2}{k_2+k_1}, \quad t_R=\frac{2k_1}{k_2+k_1},$$

$$r_L=\frac{k_2-k_1}{k_2+k_1}, \quad r_R=\frac{k_1-k_2}{k_2+k_1},$$

$$W=\frac{4ik_1k_2}{k_2+k_1}. \tag{9}$$

The flux-conserving transmission and reflection probabilities for the ideal interface are given by $T_0(E,\mathbf{k}_\parallel)=t_Lt_R$ and $R_0(E,\mathbf{k}_\parallel)=|r_L|^2=|r_R|^2$, respectively. As expected, the transmission and reflection probabilities are equivalent to forms found in standard quantum mechanics textbooks for scattering from a potential step. Techniques for calculating transmission and reflection amplitudes have also been derived for the first-principles-based layer Korringa-Kohn-Rostoker technique[14] and for the semiempirical tight-binding technique.[15]

From the above equations we see that the electron Green function can be related to the transmission or reflection amplitudes depending on whether its spatial arguments are on the same or different sides of the interface. In order to calculate the effects of interfacial disorder and roughness on the probability of transmission or reflection, it is useful to consider the quantity $F=\int d\rho'\langle G^+(\mathbf{r},\mathbf{r}')G^-(\mathbf{r}',\mathbf{r})\rangle$, the probability for an electron (at the Fermi energy) to propagate from point $\mathbf{r}$ to any point in the plane defined by z'. Here the angular brackets indicate an average over the interfacial disorder. For the case of a perfect interface this quantity can be easily evaluated to give

$$F_0=\frac{1}{4\pi^2}\int d\mathbf{k}_\parallel\int d\mathbf{k}_\parallel' G_0^+(z,z';\mathbf{k}_\parallel)G_0^-(z',z;\mathbf{k}_\parallel')\,\delta(\mathbf{k}_\parallel-\mathbf{k}_\parallel')$$

$$=\begin{cases}\left(\dfrac{m}{\pi\hbar^2}\right)^2\displaystyle\int d\mathbf{k}_\parallel\frac{T_0(\mathbf{k}_\parallel)}{4k_1(\mathbf{k}_\parallel)k_2(\mathbf{k}_\parallel)}, & \text{if } z<0,\ z'>0,\\ \left(\dfrac{m}{\pi\hbar^2}\right)^2\displaystyle\int d\mathbf{k}_\parallel\frac{1+R_0(\mathbf{k}_\parallel)+2\,\mathrm{Re}[r_Re^{-2ik_1z'}]}{4k_1^2(\mathbf{k}_\parallel)}, & \text{if } z<0,\ z'<0.\end{cases}$$

Thus F_0 can be expressed in terms of the transmission or reflection probabilities of the perfect interface divided by velocity factors that depend on the velocities in the leads. For transmission we have

$$4\pi^2 F_0 = \int d\mathbf{k}_\parallel \int d\mathbf{k}'_\parallel \frac{T_0(\mathbf{k}_\parallel,\mathbf{k}'_\parallel)\,\delta(\mathbf{k}_\parallel-\mathbf{k}'_\parallel)}{\hbar^2 v_1(\mathbf{k}_\parallel) v_2(\mathbf{k}'_\parallel)}, \quad z<0, \quad z'>0, \tag{10}$$

and (ignoring the interference terms that depend on z') for reflection,

$$4\pi^2 F_0 = \int d\mathbf{k}_\parallel \int d\mathbf{k}'_\parallel \frac{[1+R_0(\mathbf{k}_\parallel,\mathbf{k}'_\parallel)]\,\delta(\mathbf{k}_\parallel-\mathbf{k}'_\parallel)}{\hbar^2 v_1(\mathbf{k}_\parallel) v_1(\mathbf{k}'_\parallel)}, \quad z<0, \quad z'<0, \tag{11}$$

where $v_1=\hbar k_1/m$ and $v_2=\hbar k_2/m$. These results are not surprising given the known relationships between the Kubo and Landauer formulas for conductance.[28–30] At the cost of significantly greater complexity, rather than working with the quantity F, we could have worked with F' defined by

$$F' = \int d\rho' \left\langle \frac{\partial}{\partial z}\mathcal{G}(\mathbf{r},\mathbf{r}')\frac{\partial}{\partial z'}\mathcal{G}(\mathbf{r}',\mathbf{r}) + \frac{\partial}{\partial z'}\mathcal{G}(\mathbf{r},\mathbf{r}')\frac{\partial}{\partial z}\mathcal{G}(\mathbf{r}',\mathbf{r}) - \frac{\partial}{\partial z}\frac{\partial}{\partial z'}\mathcal{G}(\mathbf{r},\mathbf{r}')\mathcal{G}(\mathbf{r}',\mathbf{r}) - \mathcal{G}(\mathbf{r},\mathbf{r}')\frac{\partial}{\partial z}\frac{\partial}{\partial z'}\mathcal{G}(\mathbf{r}',\mathbf{r}) \right\rangle, \tag{12}$$

where $\mathcal{G}(\mathbf{r},\mathbf{r}')=\mathbf{G}_0^+(\mathbf{r},\mathbf{r}')-\mathbf{G}_0^-(\mathbf{r},\mathbf{r}')$. Because F' includes the current operator in its definition, it is proportional to the transmission probability (for $z<0$, $z'>0$) without the velocity factors that appear in the denominator of Eqs. (10) and (11).

In the presence of interfacial disorder or roughness, the Green function can be expanded as

$$\mathbf{G}(\mathbf{r},\mathbf{r}') = \mathbf{G}_0(\mathbf{r},\mathbf{r}') + \int d\mathbf{r}_1 \mathbf{G}_0(\mathbf{r},\mathbf{r}_1) V_i(\mathbf{r}_1)\mathbf{G}_0(\mathbf{r}_1,\mathbf{r}') + \int\int d\mathbf{r}_1 d\mathbf{r}_2 \mathbf{G}_0(\mathbf{r},\mathbf{r}_1) V_i(\mathbf{r}_1)\mathbf{G}_0(\mathbf{r}_1,\mathbf{r}_2) \times V_i(\mathbf{r}_2)\mathbf{G}_0(\mathbf{r}_2,\mathbf{r}') + \cdots, \tag{13}$$

where $G(\mathbf{r},\mathbf{r}')$ is the Green's function in the presence of interface impurities and $V_i(\mathbf{r})$ is the interface impurity potential.

In our case we have assumed that the distribution of random point scatterers and the potential $V_i(r)$ possess the following properties:

$$\langle V_i(\mathbf{r})\rangle = 0 \tag{14}$$

and

$$\langle V_i(\mathbf{r}) V_i(\mathbf{r}')\rangle = \gamma\delta(\rho-\rho')\,\delta(z)\,\delta(z'), \tag{15}$$

where the configurational average has been taken over the interface impurity potential and the correlation coefficient γ acts as a measure of the strength of the impurity scattering at the interface.

A. Specular transmission and reflection

In a condensed notation, the configurational average $\langle G^+(\mathbf{r},\mathbf{r}')G^-(\mathbf{r}',\mathbf{r})\rangle$ can be written as

$$\langle \mathbf{G}^+\mathbf{G}^-\rangle = \langle (\mathbf{G}_0^+ + \mathbf{G}_0^+ V_i \mathbf{G}_0^+ + \mathbf{G}_0^+ V_i \mathbf{G}_0^+ V_i \mathbf{G}_0^+ + \cdots) \times (\mathbf{G}_0^- + \mathbf{G}_0^- V_i \mathbf{G}_0^- + \mathbf{G}_0^- V_i \mathbf{G}_0^- V_i \mathbf{G}_0^- + \cdots)\rangle = \langle \mathbf{G}^+\rangle\langle \mathbf{G}^-\rangle + \text{vertex corrections}. \tag{16}$$

Because the configurational average restores the two-dimensional periodicity, use of the separately averaged Green functions in F yields

$$4\pi^2 F = \int d\mathbf{k}_\parallel \langle G^+(z,z';\mathbf{k}_\parallel)\rangle\langle G^-(z',z;\mathbf{k}_\parallel)\rangle, \tag{17}$$

where

$$\langle \mathbf{G}^+(\mathbf{r},\mathbf{r}';E)\rangle = \frac{1}{4\pi^2}\int d\mathbf{k}_\parallel e^{i\mathbf{k}_\parallel\cdot\rho}\langle G^+(z,z';E,\mathbf{k}_\parallel)\rangle. \tag{18}$$

Thus, use of the separately averaged Green function in F will yield expressions for the averaged transmission and reflection probabilities that depend only on a single value of $\mathbf{k}_\parallel$. These $\mathbf{k}_\parallel$-conserving terms describe specular transmission and reflection.

We can evaluate the specular transmission and reflection probabilities to lowest order within the FERPS model directly. If we take the configurational average of $G(\mathbf{r},\mathbf{r}')$, the second term in Eq. (13) drops out due to the properties of the perturbing potential [Eq. (14)] and the averaged Green's function for the system is given to lowest order by

$$\langle \mathbf{G}(\mathbf{r},\mathbf{r}')\rangle = \mathbf{G}_0(\mathbf{r},\mathbf{r}') + \int d\mathbf{r}_1 \int d\mathbf{r}_2 \langle \mathbf{G}_0(\mathbf{r},\mathbf{r}_1) V_i(\mathbf{r}_1)\mathbf{G}_0(\mathbf{r}_1,\mathbf{r}_2) \times V_i(\mathbf{r}_2)\mathbf{G}_0(\mathbf{r}_2,\mathbf{r}')\rangle. \tag{19}$$

Substituting for G_0 using Eq. (2) and for $\langle V_i(\mathbf{r}_1)V_i(\mathbf{r}_2)\rangle$ using Eq. (15) we obtain

$$\langle G(z,z';\mathbf{k}_\parallel)\rangle = G_0(z,z';\mathbf{k}_\parallel) + G_0(z,0;\mathbf{k}_\parallel)G_0(0,z';\mathbf{k}_\parallel)\frac{\gamma}{4\pi^2} \times \int d\mathbf{k}'_\parallel G_0(0,0,\mathbf{k}'_\parallel). \tag{20}$$

This form of the equation allows us to use the expressions determined earlier for the ideal interface to calculate the average Green's function. The first term in the above expression for $G(z,z';\mathbf{k}_\parallel)$ represents an electron that travels from z to z' without interacting with the impurities on the interface.

The second term accounts for electrons that travel from z, scatter from an impurity at $z=0$, and travel to z'.

We first consider the case in which z and z' are on opposite sides of the interface, $z<0$ $z'>0$. Substituting the forms for the one-dimensional Green functions from Eq. (8) we obtain

$$\langle G^+(z,z')\rangle = \frac{2m}{\hbar^2}\frac{t_R}{2ik_1}e^{-ik_1 z}e^{ik_2 z'} \times\left[1+\frac{2m}{\hbar^2}\frac{t_L}{2ik_2}\gamma\mathbf{G}_0^+(0;E)\right], \quad (21)$$

which allows us to express $\langle G^+\rangle\langle G^-\rangle$ to first order in γ as

$$\langle G^+(z,z';\mathbf{k}_\parallel)\rangle\langle G^-(z',z;\mathbf{k}_\parallel)\rangle = \left(\frac{2m}{\hbar^2}\right)^2\frac{T_0(\mathbf{k}_\parallel)}{4k_1(\mathbf{k}_\parallel)k_2(\mathbf{k}_\parallel)}\left[1+\frac{2m}{\hbar^2}\frac{t_L(\mathbf{k}_\parallel)}{2ik_2}\gamma \times[\mathbf{G}_0^+(0;E)-\mathbf{G}_0^-(0;E)]\right]. \quad (22)$$

Note that the equal-argument three-dimensional Green function that appears in Eq. (21), $\mathbf{G}_0^+(0;E)\equiv\mathbf{G}_0(\mathbf{r},\mathbf{r};E)$ where $\mathbf{r}$ lies at the interface, is formally divergent. This problem is inherent in the random δ-function model in three dimensions and can be avoided by considering scattering from scatterers with small but finite size or by cutting off the divergent integral over momentum at a value k_{max} which is on the order of the size of the scatterers.[31] The divergence, however, does not affect the imaginary part of the equal-argument Green function which appears in Eq. (22) and represents the density of states at the interface:

$$\mathbf{G}_0^+(0;E)-\mathbf{G}_0^-(0;E) = \frac{1}{3\pi i}\frac{2m}{\hbar^2}\left(\frac{k_1(0)^3-k_2(0)^3}{k_1(0)^2-k_2(0)^2}\right) = -2\pi i\, n_0(0;E), \quad (23)$$

where $\hbar k_1(0)=\sqrt{2m(E-U_1)}$ and $\hbar k_2(0)=\sqrt{2m(E-U_2)}$. Thus the specular part of the transmission probability for the disordered interface, $T(\mathbf{k}_\parallel)$, can be written as the transmission probability for the ideal interface multiplied by a factor that depends on $\mathbf{k}_\parallel$. This dependence on $\mathbf{k}_\parallel$ can, of course, be translated into a dependence on the angle of incidence:

$$T(\mathbf{k}_\parallel)=T_0(\mathbf{k}_\parallel)S_t(\mathbf{k}_\parallel)=T_0(\mathbf{k}_\parallel)\left(1-\frac{4\pi}{\hbar}\frac{\gamma n_0(0;E)}{v_1(\mathbf{k}_\parallel)+v_2(\mathbf{k}_\parallel)}\right). \quad (24)$$

Here $v_1(\mathbf{k}_\parallel)$ and $v_2(\mathbf{k}_\parallel)$ are the z components of electron velocity in each material for a given $\mathbf{k}_\parallel$. The specularity factor for transmission at the rough interface is given by $S_t(\mathbf{k}_\parallel)$. The transmission equation derived above is similar to expressions for point scatterers at an interface previously derived using wave function boundary matching conditions.[32,33]

Within the FERPS model, the reduction of specular transmission due to diffuse scattering is smallest at normal incidence and increases as the normal components of the velocity on either side of the interface become small. Since the second term is always positive, diffusive scattering from the interface can only reduce the transmission probability of electrons (at least within lowest-order perturbation theory). The apparent singularity in the specularity parameter for $v_1(\mathbf{k}_\parallel)\to 0$, especially when $v_1(\mathbf{k}_\parallel)=v_2(\mathbf{k}_\parallel)$, which makes it appear that S_t might become negative is an artifact of our use of lowest-order perturbation theory. When higher-order terms in the dimensionless parameter $\gamma n_0/(\hbar v_F)$ are included as described in the Appendix (and the artificial divergence caused by the use of point impurities is handled) the specular transmission and reflection probabilities are never negative.

We can obtain the probability for specular reflection by evaluating F for the case in which the Green function arguments z and z' are on the same side of the interface. The Green's function in this case is given by

$$G_0^+(z,z';\mathbf{k}_\parallel)=G_0^{+L}(z,z';\mathbf{k}_\parallel)+\frac{r_R}{2ik_1}e^{-ik_1(z+z')}, \quad (25)$$

where $G_0^{+L}(z,z';\mathbf{k}_\parallel)$ is the Green function for an infinite medium with properties of the material on the left side. For this case $\langle G^+(z,z';\mathbf{k}_\parallel)\rangle$ is given to first order in γ by

$$\langle G^+(z,z';\mathbf{k}_\parallel)\rangle = \frac{2m}{\hbar^2}\frac{e^{-ik_1 z}e^{ik_1 z'}}{2ik_1}+\frac{2m}{\hbar^2}\frac{e^{-ik_1 z}e^{-ik_1 z'}}{2ik_1} \times\left(r_R+\frac{2m}{\hbar^2}\frac{(1+r_R)^2}{2ik_1}\gamma\mathbf{G}^+(0;E)\right). \quad (26)$$

In this form, we see that the reflection amplitude r_R is effectively modified by the presence of the impurity scattering leading to an effective reflection amplitude $\overline{r_R}$ given by

$$\overline{r_R}=r_R+\frac{2m}{\hbar^2}\frac{(1+r_R)^2}{2ik_1}\gamma\mathbf{G}^+(0;E). \quad (27)$$

Although this form contains the divergent equal-argument Green function, the lowest-order expression for the reflection probability again contains only the well-defined imaginary part

$$R(\mathbf{k}_\parallel)=R_0(\mathbf{k}_\parallel)-\frac{8\pi}{\hbar}\frac{v_1(\mathbf{k}_\parallel)[v_1(\mathbf{k}_\parallel)-v_2(\mathbf{k}_\parallel)]}{[v_1(\mathbf{k}_\parallel)+v_2(\mathbf{k}_\parallel)]^3}\gamma n_0(0;E). \quad (28)$$

The expression for the effective reflectivity $R(\mathbf{k}_\parallel)$ can also be expressed in terms of a specularity constant for reflection and the reflection probability for an ideal interface. This is given as

$$R(\mathbf{k}_\parallel)=S_r(\mathbf{k}_\parallel)R_0(\mathbf{k}_\parallel), \quad (29)$$

where $S_r(\mathbf{k}_\parallel)$ is given by

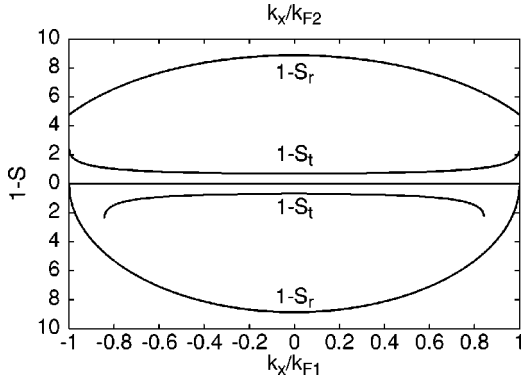

FIG. 2. $1-S_t$ and $1-S_r$ in the FERPS model. The Fermi momentum k_{F1} corresponds to 0.5 electrons per spin channel (e.g., as in Cu) while k_{F2} corresponds to 0.3 electrons per spin channel (e.g., as in majority Co). The values of $1-S_t$ and $1-S_r$ are measured in terms of the dimensionless parameter $2m_e\gamma n_0 a/\hbar^2$, where a is the lattice constant for an assumed fcc lattice.

$$S_r(\mathbf{k}_\parallel)=1-\frac{8\pi}{\hbar}\frac{v_1(\mathbf{k}_\parallel)}{v_1^2(\mathbf{k}_\parallel)-v_2^2(\mathbf{k}_\parallel)}\gamma n_0(0;E). \tag{30}$$

Again, the apparent singularity for a symmetric interface which makes it appear that S_r might become negative is an artifact of our use of lowest-order perturbation theory. It is shown in the Appendix that S_r is always greater than zero.

A few general observations may be made concerning the specularity functions for reflection and transmission within the FERPS model: (1) The relative effect of diffuse scattering on the reflected beam can be much larger than its effect on the transmitted beam,

$$\frac{1-S_r(\mathbf{k}_\parallel)}{1-S_t(\mathbf{k}_\parallel)}=\frac{2v_1(\mathbf{k}_\parallel)}{v_1(\mathbf{k}_\parallel)-v_2(\mathbf{k}_\parallel)}, \tag{31}$$

especially when $v_1(\mathbf{k}_\parallel)\approx v_2(\mathbf{k}_\parallel)$. (2) For the case of transmission, increased surface roughness can only reduce specular transport across the interface, whereas for the case of reflection, interfacial disorder can either increase or decrease the specular reflection depending on the electron velocities for each material at a particular value of $\mathbf{k}_\parallel$. This model actually predicts that interfacial disorder *increases* the specularly reflected flux for $v_2(\mathbf{k}_\parallel)>v_1(\mathbf{k}_\parallel)$. (3) Specular transmission remains symmetric in the sense that transmission from left to right remains the same as from right to left. Specular reflection, however, is no longer symmetric in the presence of a disordered interface.

The specularity parameters are plotted both as functions of $k_\parallel/k_{F1}$ and $k_\parallel/k_{F2}$ in Fig. 2. Note that within this model the diffuse scattering in reflection vanishes as $k_\parallel\to k_{F1}$ where $k_{F1}>k_{F2}$. Generally, however, the model predicts the effects of diffuse scattering to be significantly greater for the reflected beam than for the transmitted beam. The range of k_x/k_{F1} for which no values are given for $1-S_t$ corresponds to the values of $\mathbf{k}_\parallel$ which yield total reflection; that is, there is no specular transmission probability because the transmitted waves are evanescent.

The total flux removed from the specular beams by the interfacial disorder is given by

$$F_d=\frac{4\pi}{\hbar}\gamma n_0(0;E)\frac{2v_1(\mathbf{k}_\parallel)}{[v_1(\mathbf{k}_\parallel)+v_2(\mathbf{k}_\parallel)]^2}. \tag{32}$$

This flux must reappear as diffuse flux if current is to be conserved.

B. Diffuse scattering

In addition to the specular part of the transmitted and reflected fluxes, there will be diffusely scattered electrons. The transmission and reflection probabilities for diffuse scattering can be obtained from the $\mathbf{k}_\parallel$ nonconserving contributions to $\langle G^+G^-\rangle$. For the simple model of free electrons with random point scattering this is given in lowest order by $\langle G_0^+VG_0^+G_0^-VG_0^-\rangle$. Thus the lowest-order vertex correction to F is given by

$$\begin{aligned}F_{vc}=&\int d\rho' d\rho_1 d\rho_2\left(\frac{1}{4\pi^2}\right)^2\int d\mathbf{k}_\parallel d\mathbf{k}'_\parallel d\mathbf{k}''_\parallel d\mathbf{k}'''_\parallel \gamma\delta(\rho_1-\rho_2)\\&\times\delta(z_1)\delta(z_2)e^{i\mathbf{k}_\parallel\cdot(\rho-\rho_1)}e^{i\mathbf{k}'_\parallel\cdot(\rho_1-\rho')}e^{i\mathbf{k}''_\parallel\cdot(\rho'-\rho_2)}\\&\times e^{i\mathbf{k}'''_\parallel\cdot(\rho_2-\rho)}G_0^+(\mathbf{k}_\parallel,z,z_1)G_0^-(\mathbf{k}'_\parallel,z_1,z')\\&\times G_0^+(\mathbf{k}''_\parallel,z',z_2)G_0^-(\mathbf{k}'''_\parallel,z_2,z).\end{aligned} \tag{33}$$

This can be evaluated to yield

$$\begin{aligned}F_{vc}=&\frac{\gamma}{16\pi^4}\left(\frac{2m}{\hbar^2}\right)^4\int d\mathbf{k}_\parallel\int d\mathbf{k}'_\parallel\\&\times\frac{1}{[k_1(\mathbf{k}_\parallel)+k_2(\mathbf{k}_\parallel)]^2}\frac{1}{[k_1(\mathbf{k}'_\parallel)+k_2(\mathbf{k}'_\parallel)]^2}.\end{aligned} \tag{34}$$

Comparison with Eq. (10) allows us to write the diffuse contribution to the transmission as

$$\begin{aligned}&T_{vc}(\mathbf{k}_\parallel,\mathbf{k}'_\parallel)\\&\quad=\frac{16\gamma}{4\pi^2\hbar^2}\frac{v_1(\mathbf{k}_\parallel)}{[v_1(\mathbf{k}_\parallel)+v_2(\mathbf{k}_\parallel)]^2}\frac{v_2(\mathbf{k}'_\parallel)}{[v_1(\mathbf{k}'_\parallel)+v_2(\mathbf{k}'_\parallel)]^2}.\end{aligned} \tag{35}$$

Similarly, the diffuse contribution to reflection is given by

$$\begin{aligned}&R_{vc}(\mathbf{k}_\parallel,\mathbf{k}'_\parallel)\\&\quad=\frac{16\gamma}{4\pi^2\hbar^2}\frac{v_1(\mathbf{k}_\parallel)}{[v_1(\mathbf{k}_\parallel)+v_2(\mathbf{k}_\parallel)]^2}\frac{v_1(\mathbf{k}'_\parallel)}{[v_1(\mathbf{k}'_\parallel)+v_2(\mathbf{k}'_\parallel)]^2}.\end{aligned} \tag{36}$$

The total diffuse flux

$$F_d = \int d\mathbf{k}_\parallel' [T_{vc}(\mathbf{k}_\parallel, \mathbf{k}_\parallel') + R_{vc}(\mathbf{k}_\parallel, \mathbf{k}_\parallel')] \tag{37}$$

is easily seen to be equal to the missing specular flux given in Eq. (32).

For the particular case of the FERPS model, the transmission and reflection depend only on the magnitude of $\mathbf{k}_\parallel$ and $\mathbf{k}_\parallel'$. Thus the expressions for the transmission and reflection can be simplified for visualization as

$$T_{vc}(x,y) = \frac{16\gamma}{h^2 v_{F1} v_{F2}} \frac{\sqrt{1-x^2}}{(\sqrt{1-x^2}+\sqrt{a^2-x^2})^2} \frac{\sqrt{1-y^2}}{(\sqrt{1-y^2}+\sqrt{a^{-2}-y^2})^2}, \tag{38}$$

where $x = k_\parallel / k_{F1}$, $y = k_\parallel' / k_{F2}$, and $a = k_{F2}/k_{F1}$. For $k_\parallel > k_{F2}$ (equivalent to $x > a$), the Green functions in Eq. (33) yield

$$T_{vc}(x,y) = \frac{16\gamma}{h^2 v_{F1} v_{F2}} \frac{\sqrt{1-x^2}}{1-a^2} \frac{\sqrt{1-y^2}}{(\sqrt{1-y^2}+\sqrt{a^{-2}-y^2})^2}. \tag{39}$$

Similarly, the diffuse reflection probability can be simplified for visualization as

$$R_{vc}(x,y) = \frac{16\gamma}{h^2 v_{F1}^2} \frac{\sqrt{1-x^2}}{(\sqrt{1-x^2}+\sqrt{a^2-x^2})^2} \frac{\sqrt{1-y^2}}{(\sqrt{1-y^2}+\sqrt{a^2-y^2})^2}, \tag{40}$$

where $x = k_\parallel / k_{F1}$, $y = k_\parallel' / k_{F1}$, and $a = k_{F2}/k_{F1}$. For x or y greater than a, the denominator again becomes $1-a^2$.

Figure 3 shows plots of the diffuse scattering as a function of $k_\parallel$ and $k_\parallel'$ for transmission and reflection. The interface considered in this particular example is appropriate to a free electron model for the majority copper-cobalt interface, i.e., Fermi surfaces containing 0.5 electrons/atom (Cu) and 0.3 electrons/atom (Co). The diffuse transmission [panel (a)] is symmetric in terms of whether the electron is incident from the larger (k_{F1}) or smaller (k_{F2}) Fermi surface. The diffuse transmission can be seen to be fairly uniform over much of $k_\parallel$-$k_\parallel'$ space. On the side of the interface with the smaller Fermi surface, there is a small maximum for relatively large values of $k_\parallel'$ before it vanishes at $k_\parallel' = k_{F2}$. On the side of the interface with the larger Fermi surface, there is a large maximum with discontinuous slope at the largest value of $k_\parallel$ for which specular transmission is possible. For still larger values of $k_\parallel$, there is a region for which diffuse transmission is possible, but not specular transmission. In this region the diffuse transmission rapidly decreases to zero (with infinite slope) at $k_\parallel = k_{F1}$. Thus interfacial disorder allows transmission of electrons with an incident $k_\parallel$ (on the larger Fermi surface) that would normally be totally reflected and also allows scattering into values of $k_\parallel$ on the larger Fermi surface that are not accessible to specular transmission. For the pointlike disorder considered here there is no evidence for enhancement of diffuse scattering near the forward scattering direction ($\mathbf{k}_\parallel = \mathbf{k}_\parallel'$).

The diffuse reflection probability depends on whether the electron is incident on the larger Fermi surface or the smaller. For electrons incident from the material with the smaller Fermi surface [panel (c)] the diffuse scattering is

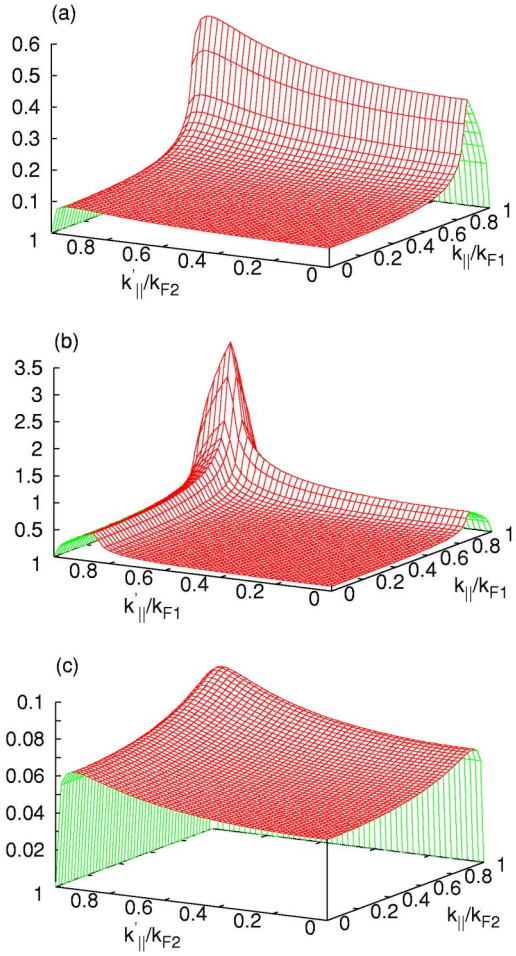

FIG. 3. (Color online) Calculated diffuse scattering in transmission (a) and reflection (b) and (c). Plotted values are dimensionless and should be multiplied by $16\gamma/h^2 v_{F1} v_{F2}$ (transmission) or $16\gamma/h^2 v_{F1}^2$ (reflection). For panel (b) electrons are incident from the larger Fermi surface and for panel (c) from the smaller.

relatively smooth and uniform with a weak maximum before vanishing when either the incident or reflected $k_\parallel$ equals k_F. For electrons incident from the larger Fermi surface [panel (b)] there is a maximum in the diffuse reflection probability for the value of $k_\parallel$ or $k_\parallel'$ for the critical angle at which total reflection begins for the specular beam. This maximum comes from the same source [vanishing of $v_2(k_\parallel)$] in Eq. (33) as the maximum in the transmitted diffuse scattering.

III. LKKR-CPA CALCULATIONS

In this section, the LKKR method will be used to calculate the probability for specular transmission and reflection across an interface for the case of a more realistic model that should be appropriate for certain real interfaces such as those that are formed by sputter or ion beam deposition of layers of cobalt and copper. In the previous section, we showed that the specular transmission and reflection probabilities for electrons incident on an atomically disordered interface can be obtained from the configuration-averaged Green function. This is a quantity that the coherent potential approximation[25–27] is designed to calculate. Thus, we can use the LKKR technique to obtain the average Green function in the coherent potential approximation for the disordered interface and then calculate the transmission and reflection probabilities using this averaged Green function.[14] This should approximate the specular transmission and reflection probabilities in the presence of the assumed interfacial disorder. For both the free electron and real material interfaces, the specularity functions for transmission and reflection are determined using the following equations:

$$S_t(\mathbf{k}_\parallel) = \frac{T_{cpa}(\mathbf{k}_\parallel)}{T_0(\mathbf{k}_\parallel)},$$

$$S_r(\mathbf{k}_\parallel) = \frac{R_{cpa}(\mathbf{k}_\parallel)}{R_0(\mathbf{k}_\parallel)}, \tag{41}$$

where $T_{cpa}(\mathbf{k}_\parallel)$ and $R_{cpa}(\mathbf{k}_\parallel)$ are the transmission and reflection probabilities in the CPA case and $T_0(\mathbf{k}_\parallel)$ and $R_0(\mathbf{k}_\parallel)$ are similar quantities for the ordered interface.

In order to make contact with the results of the previous section we shall begin with a calculation that mimics the free electron calculations of that section within the context of the LKKR approach. Thus we assume, as in the last section, that the electronic structure on either side of the interface is that of free electrons. Within the LKKR approach which utilizes the atomic sphere approximation, a uniform potential is approximated by a superposition of uniform potentials within slightly overlapping atomic spheres of volume equal to the volume per atom. Thus our LKKR approximation to the disordered interface consists of atomic spheres of uniform potential $+U$ on the left of the interface and uniform potential $-U$ on the right of the interface. Each of these is arranged on a semi-infinite fcc lattice with the interface perpendicular to the (100) direction. The interface consists of a single fcc (100) layer of atomic spheres randomly occupied by $+U$ or $-U$ "atoms." In the LKKR approach (as in a real system) the disordered interface must have a finite width equal to that of at least one atomic layer.

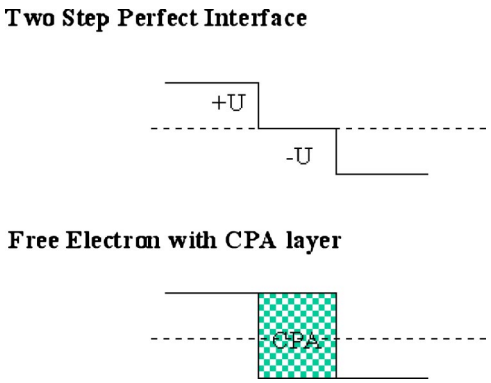

FIG. 4. (Color online) Two separate interfaces are used when studying interface scattering for free electrons. The first interface is a double potential step that has an intermediate potential level at the interface equal to the average of the two bulk potentials. In the LKKR calculation, this potential region is approximated as a CPA alloy layer.

$T_0(\mathbf{k}_\parallel)$ and $R_0(\mathbf{k}_\parallel)$ are calculated by replacing the atomic layer of $+U$ and $-U$ potentials with an atomic layer of $U=0$ potentials as required by Eq. (14) (Fig. 4). The lattice spacings and atomic sphere radii are appropriate to a copper lattice [layer thickness of 3.4083 a.u., the width of one atomic layer of copper or cobalt in the (100) direction]. The potentials on the left and right sides of the step are given by $+U$ and $-U$, respectively, where $U=0.050$ Ry. The free electron energy was taken to be 0.664 Ry (corresponding approximately to the Fermi energy of copper).

The results of the LKKR-CPA calculation for the transmission specularity parameter S_t are compared to the analytic results derived in the previous section in Fig. 5. We find remarkably good agreement between the LKKR-CPA approach and the analytic Green's function technique, espe-

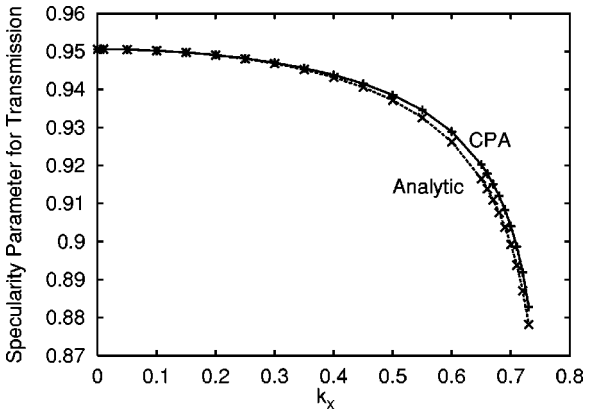

FIG. 5. The specularity parameter for transmission calculated for the free electron interface shows good agreement between the analytical Green function (dotted line with crosses) and LKKR-CPA (solid line with "+" symbols) approaches. The momentum states in which $k_y=0$ and k_x is allowed to vary were considered. Units for k_x are a.u.$^{-1}$. In this case, $U=0.05$ Ry and $\gamma_{fit}=0.292$ Ry^2 a.u.^{4}.

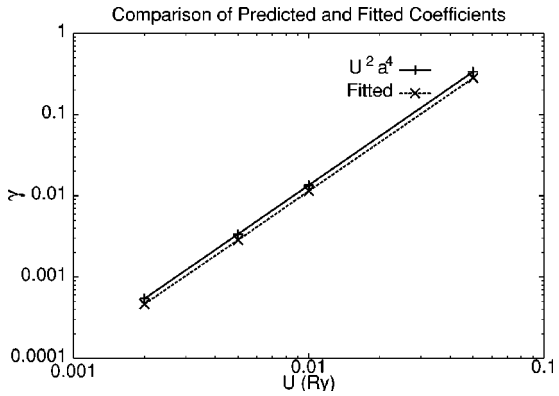

FIG. 6. The fitted parameter γ which measures the strength of the interfacial potential scattering in the FERPS model and U^2a^4 are plotted as a function of U, the interfacial potential used in the CPA.

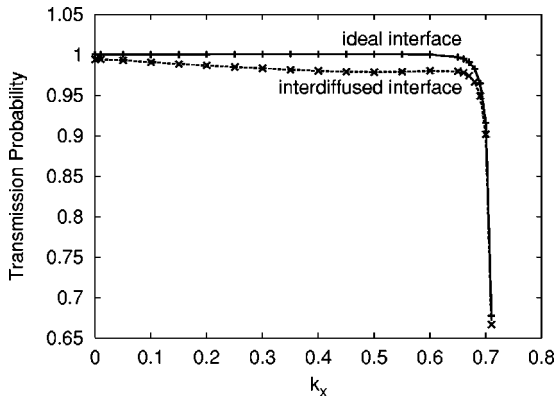

FIG. 7. Transmission is shown for a sharp and interdiffused (100) Co|Cu interface. Transmission for the perfect interface is represented by a solid line with crosses (+). A dashed line with symbols (×) is used for transmission across an interdiffused interface modeled as a $Co_{50}Cu_{50}$ alloy layer. In the case of the interdiffused interface, there is enhanced diffusive scattering for higher $\mathbf{k}_\parallel$ and a significant drop in overall transmission. Units for k_x are a.u.$^{-1}$.

cially considering the fact that the LKKR method must approximate the uniform potential by a sum of spherical potentials. In agreement with the analytic results, the transmission specularity parameter decreases rapidly as the z component of the electron momentum or velocity becomes small.

The analytical Green's function specularity parameter fits the specularity parameter for transmission in the LKKR-CPA case using a correlation parameter $\gamma = 0.292$ Ry^2 a.u.^{4} for $U = 0.05$ Ry. This is quite close to the estimate for γ based on dimensional arguments, $\gamma = U^2a^4 = 0.334$ Ry^2 a.u.^{4}, where a is the step size. Figure 6 shows that γ fitted to the transmission specularity parameter is approximately $0.87U^2a^4$ over a large range in the potential step U.

Interfacial scattering at a (100) interface in a Co|Cu bilayer is also considered using the LKKR-CPA technique. In this approach, the electronic structure of the entire interface region is calculated self-consistently. This interface region consists of 16 atomic layers that are allowed to relax in the process of achieving electronic self-consistency. During the self-consistency process, these interfacial layers are surrounded by semi-infinite bulk copper adjacent to the relaxed copper and by semi-infinite bulk cobalt adjacent to the relaxed cobalt.

It is assumed that the diffusive scattering arises from interdiffusion of the two materials on the scale of a few atomic layers. We therefore model the interface as having a small number of atomic layers in which the atoms are randomly Co or Cu. The electronic structure of these layers is calculated using the coherent potential approximation. In order to provide a computational estimate of the $\mathbf{k}_\parallel$-dependent S parameter, the transmission and reflection probabilities of two systems are calculated, a Co|Cu interface with no interdiffusion and an interface with one or more layers of Co_xCu_{1-x} alloy.

Figure 7 shows the transmission probability calculated for a sharp (no interdiffusion) interface and the specular transmission probability for an interface modeled with a single atomic layer of composition $Co_{0.5}Cu_{0.5}$. The majority channel was chosen for this example because it has only one Bloch state for most $\mathbf{k}_\parallel$ points in both Co and Cu and might, therefore, be expected to have some similarity to the FERPS model. Transmission in both cases drops as the momentum parallel to the interface increases and momentum perpendicular to the interface vanishes. It should be noted, however, that due to the close matching of the bands for majority Co and Cu, the overall transmission is still extremely high for most values of k_x.

Figure 8 shows the specular transmission and reflection probabilities on a logarithmic scale for the majority cobalt-copper (100) interface as a function of the degree of interfacial intermixing. Two features are surprising about Fig. 8. In the absence of intermixing the transmission probability is nearly unity and the reflection probability nearly zero over most of the range of $k_\parallel$. For comparison, a free electron model for the ideal cobalt-copper interface with T and R calculated from Eqs. (9) assuming Fermi sphere volumes of 0.3 and 0.5 electrons/atom, respectively, would give a reflection probability at least 30 times larger than that shown in Fig. 8 for most values of $k_\parallel$.

In the absence of intermixing, $R = 1 - T$. At the lowest values of intermixing that we considered (0.1%), $1 - T$ is very slightly greater than R. In addition to diffuse scattering, the difference between R and $1 - T$ seen in Fig. 8 for the lowest intermixing may be due to numerical inaccuracies that arise primarily because the T and R matrices are calculated using Green functions that have a small imaginary part to the energy. This is needed to maintain their correct analytic behavior. The increase in reflection for large $k_\parallel$ is due to the Fermi surface of copper being larger than that of majority cobalt so that total reflection occurs when for a given value of $k_\parallel$ there is no cobalt state for the electron to be refracted into.

The second surprising feature is that substantial intermixing of two atomic layers has only a small effect on the transmission and reflection probabilities. The structure in the reflection probability probably results from interference within the disordered layers which have a finite thickness.

One feature of the specular transmission and reflection probability that deserves special comment is the prediction

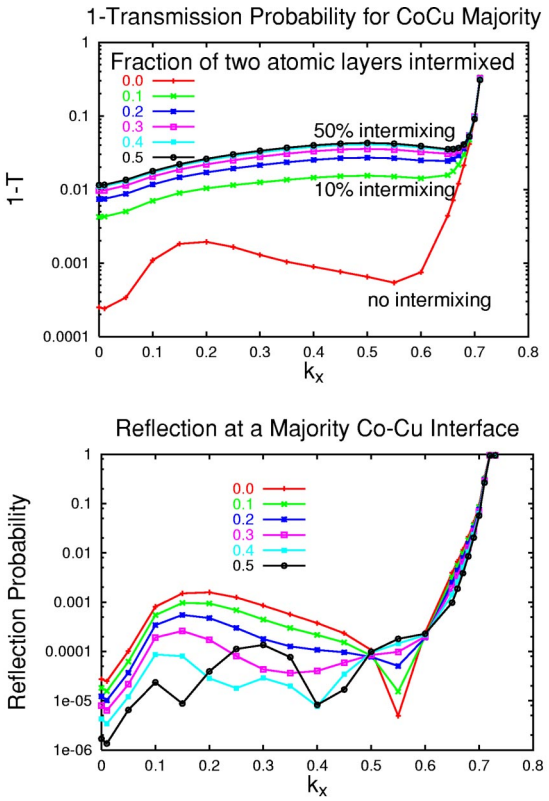

FIG. 8. (Color online) Majority channel specular transmission (subtracted from unity) and specular reflection probabilities for an interface between fcc cobalt and copper calculated in the coherent potential approximation. There are two intermixed atomic layers, one with Cu_xCo_{1-x} on the cobalt side of the interface and one with Co_xCu_{1-x} on the copper side where $x=0.1,\ldots,0.5$. The interface is assumed to be perpendicular to the (100) direction.

that atomic-scale impurities are relatively ineffective in causing diffuse scattering of electrons with sufficiently high $\mathbf{k}_\parallel$ ($k_x>0.7$ in this case) that they undergo total internal reflection. In this regard the first-principles results appear to differ qualitatively from those of the FERPS model. This observation should encourage strategies aimed at increasing current in the plane–GMR by enhancing the channeling effect in which electrons become trapped in the low-resistivity copper layer for parallel alignment of the moments, thus increasing the GMR effect.[34] Another feature of the calculated specular reflection probability that should be noted is the prediction that for certain values of $\mathbf{k}_\parallel$, diffuse scattering can actually increase the probability for specular reflection. This result is consistent with the FERPS model results.

Figure 9 shows the transmission specularity parameter for majority cobalt copper which may be compared with that for the free electrons with random point interfacial scatterers model shown in Fig. 2. One important difference is the vanishing of the effect of diffuse scattering for electrons incident on the interface with the highest values of transverse momentum, i.e., grazing incidence.

Figure 10 shows the calculated transmission and reflection probabilities for minority electrons at a cobalt-copper interface. The reflection probability can be viewed as the probability of an electron in copper being reflected off of the

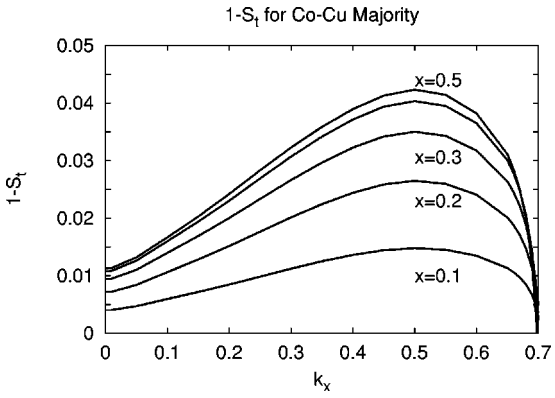

FIG. 9. $1-S_t$ for majority cobalt copper. The fraction of intermixing of two interfacial layers is indicated by x. (See caption to Fig. 8.)

interface. Because the minority spin channel for cobalt has multiple bands for most values of $k_\parallel$, the transmission probability can be viewed as the total probability that an electron in copper will be transmitted into any of the bands with the same value of $k_\parallel$. It is interesting that these calculations predict that disorder can actually increase the transmission for a few values of $k_\parallel$ for which the transmission of the ordered interface is particularly low and can increase the specular reflection for values of $k_\parallel$ where it is especially low.

One of the important results of Figs. 8 and 10 is that for most values of $k_\parallel$ the transmission probability is much higher in the majority channel than for the minority channel. In

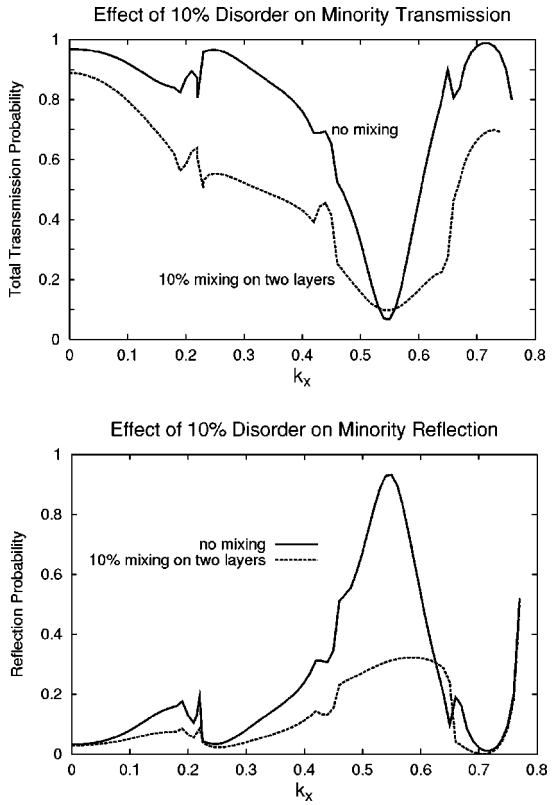

FIG. 10. Specular transmission and reflection probabilities for the minority cobalt-copper interface.

addition, the effects of disorder are not nearly so dramatic on the majority transmission as on the minority. This difference is one of the major contributors to the GMR effect and is due to the relatively good matching of the electronic structures of cobalt and copper in the majority channel and the relatively poor match in the minority channel.

IV. CONCLUSION

With the emergence of devices which rely on transport across nanoscale interfaces, a clear understanding of scattering events and interdiffusion in this region is essential. In this study, we have demonstrated that the specular part of the transmission and reflection probabilities can be obtained from the averaged single-particle Green function. The specularity parameter is demonstrated to be rather strongly dependent on $\mathbf{k}_\parallel$ or equivalently on the angle of incidence of the electron as it approaches the interface. For systems that approximate free electrons such as the majority spin channel of Co|Cu, the specularity parameter is highest for normal incidence.

The derived results for the FERPS model clearly show that the cases of reflection and transmission possess different specularity parameters. This has direct implications for semiclassical Boltzmann transport models of magnetic multilayers. Depending on the band structure of the two materials, diffuse scattering can lead to either enhanced or reduced specular reflection. Within the FERPS model, however, interdiffusion always reduces specular transmission across interfaces.

The layer KKR-CPA approach provides the ability to numerically approximate the specularity parameter for a realistic model of material interfaces. Results for a (100) Co|Cu interface provide an example which may illustrate some general trends for scattering due to interfacial interdiffusion. Depositions which result in greater interdiffusion will lead to increased diffusive scattering, reducing the specularity parameter for transmission. For the FERPS model and for (100) Co|Cu, the specularity parameter for transmission also increases for high values of $k_\parallel$. This is most likely due to the reduction of electron velocities near the Brillouin zone edge.

This work provides the tools necessary to build a semiclassical model that incorporates *ab initio* band structure information including a reasonable model of interface scattering. Recently molecular dynamics models have been able to determine the degree of interdiffusion for different deposition conditions.[6] Using the composition profiles obtained from these calculations, the LKKR-CPA model should provide accurate specularity parameters for different deposition conditions. It is hoped that these issues can be addressed in an upcoming work. Another issue that is dealt with here formally (Appendix) and in the section on the FERPS model, but not from first principles, is the full angular dependence of the diffuse scattering. We also hope to address this problem soon by developing a first-principles approach that would sum the ladder diagrams for the vertex corrections. This approach would be similar to the techniques that have been applied to homogeneous systems.[35,36]

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APPENDIX

In order to go beyond second-order perturbation theory within the FERPS model, it is convenient to consider the Green function expansion in the $\mathbf{k}_\parallel$ representation. Defining the $\mathbf{k}_\parallel$ representations for the Green's function in the presence of the interface impurity potential $V_i(\mathbf{r})=V_i(\rho)\delta(z)$ and for an ideal interface as

$$G^+(\mathbf{r},\mathbf{r}';E)=\frac{1}{A}\sum_{\mathbf{k}_{||}\mathbf{k}_{||}'} e^{i(\mathbf{k}_{||}\cdot\rho-\mathbf{k}_{||}'\cdot\rho')}G^+(z,z';E,\mathbf{k}_{||},\mathbf{k}_{||}') \tag{A1}$$

and

$$G_0^+(\mathbf{r},\mathbf{r}';E)=\frac{1}{A}\sum_{\mathbf{k}_{||}} e^{i\mathbf{k}_{||}\cdot(\rho-\rho')}G_0^+(z,z';E,\mathbf{k}_{||}), \tag{A2}$$

respectively, where $\rho=x\hat{x}+y\hat{y}$ is a two-dimensional vector in the plane of the interface with area A, we can rewrite the expansion for the Green's function in the following way (suppressing the energy argument E for brevity):

$$G(z,z';\mathbf{k}_{||},\mathbf{k}_{||}')=G_0(z,z';\mathbf{k}_{||})\delta_{\mathbf{k}_{||}\mathbf{k}_{||}'} + G_0(z,0;\mathbf{k}_{||})T(\mathbf{k}_{||},\mathbf{k}_{||}')G_0(0,z';\mathbf{k}_{||}'). \tag{A3}$$

Here the scattering T matrix (which should not be confused with the transmission probability) is

$$\begin{aligned}T(\mathbf{k}_{||},\mathbf{k}_{||}')&=V_i(\mathbf{k}_{||}-\mathbf{k}_{||}')\\&+\sum_{\mathbf{k}_{||}''}V_i(\mathbf{k}_{||}-\mathbf{k}_{||}'')G_0(0,0;\mathbf{k}_{||}'')V_i(\mathbf{k}_{||}''-\mathbf{k}_{||}')\\&+\sum_{\mathbf{k}_{||}''\mathbf{k}_{||}'''}V_i(\mathbf{k}_{||}-\mathbf{k}_{||}'')G_0(0,0;\mathbf{k}_{||}'')V_i(\mathbf{k}_{||}''-\mathbf{k}_{||}''')\\&\times G_0(0,0;\mathbf{k}_{||}''')V_i(\mathbf{k}_{||}'''-\mathbf{k}_{||}')+\cdots\end{aligned} \tag{A4}$$

and

$$V_i(\mathbf{k}_{||}-\mathbf{k}'_{||})=\frac{1}{A}\int d\rho e^{-i(\mathbf{k}_{||}-\mathbf{k}'_{||})\cdot\rho}V_i(\rho) \tag{A5}$$

is the matrix element of the interface impurity potential. $G_0(z,z';\mathbf{k}_{\|})$ is the interface Green function which is diagonal in $\mathbf{k}_{\|}$ space and which describes electron transmission through an ideal (defect free) interface. It is defined by Eqs. (8) and (9).

We need to determine the electron's probability of transmission through and reflection from a disordered interface. These can be expressed by means of the square modulus of the propagator defined in Eq. (A3) averaged over the interfacial disorder, $\langle|G(z,z';\mathbf{k}_{||},\mathbf{k}'_{||})|^2\rangle$. Let us consider, e.g., the transmission probability. In this case, the Green's function $G_0^+(z,z';\mathbf{k}_{||})$ is defined by the first two expressions of Eq. (8) (for $z<0,z'>0$ or $z>0,z'<0$) and $|G(z,z';\mathbf{k}_{||},\mathbf{k}'_{||})|^2=|G(0,0;\mathbf{k}_{||},\mathbf{k}'_{||})|^2$ does not depend on z and z'. Thus, $\langle|G(z,z';\mathbf{k}_{||},\mathbf{k}'_{||})|^2\rangle$ defining the transmission probability may be written as

$$\begin{aligned}\langle|G(\mathbf{k}_{||},\mathbf{k}'_{||})|^2\rangle=&|\langle G(\mathbf{k}_{||},\mathbf{k}'_{||})\rangle|^2\\&+\sum_{\mathbf{k}''_{||}\mathbf{k}'''_{||}}|\langle G(\mathbf{k}_{||},\mathbf{k}''_{||})\rangle|^2W(\mathbf{k}''_{||},\mathbf{k}'''_{||})\\&\times|\langle G(\mathbf{k}'''_{||},\mathbf{k}'_{||})\rangle|^2,\end{aligned} \tag{A6}$$

where $G(\mathbf{k}_{||},\mathbf{k}'_{||})=G(0,0;\mathbf{k}_{||},\mathbf{k}'_{||})$ and $W(\mathbf{k}_{||},\mathbf{k}'_{||})$ is the vertex function.

On the other hand, using Eq. (A3), we get

$$\begin{aligned}\langle|G(\mathbf{k}_{||},\mathbf{k}'_{||})|^2\rangle=&|G_0(\mathbf{k}_{||})|^2\delta_{\mathbf{k}_{||}\mathbf{k}'_{||}}\\&+|G_0(\mathbf{k}_{||})|^2 2\,\mathrm{Re}[\langle T^+(\mathbf{k}_{||},\mathbf{k}_{||})\rangle\\&\times G_0^+(\mathbf{k}_{||})]\delta_{\mathbf{k}_{||}\mathbf{k}'_{||}}\\&+|G_0(\mathbf{k}_{||})|^2\langle|T(\mathbf{k}_{||},\mathbf{k}'_{||})|^2\rangle|G_0(\mathbf{k}'_{||})|^2,\end{aligned} \tag{A7}$$

where

$$G_0^+(\mathbf{k}_{||})=G_0^+(\mathbf{k}_{||},\mathbf{k}_{||})=\frac{2}{i\hbar[v_1(\mathbf{k}_{||})+v_2(\mathbf{k}_{||})]} \tag{A8}$$

and

$$v_1(\mathbf{k}_{||})=\frac{\hbar}{m}\sqrt{\frac{2m}{\hbar^2}(E-U_1)-\mathbf{k}_{||}^2}$$

and

$$v_2(\mathbf{k}_{||})=\frac{\hbar}{m}\sqrt{\frac{2m}{\hbar^2}(E-U_2)-\mathbf{k}_{||}^2}$$

are the normal components of the electron velocity on either side of the interface. Note that the averaged Green's function $\langle G(\mathbf{k}_{||},\mathbf{k}'_{||})\rangle$ is diagonal and, therefore, according to Eq. (A3), the averaged T matrix is also diagonal.

To separate the specular and diffuse scatterings, it is useful to represent $\langle|T(\mathbf{k}_{||},\mathbf{k}'_{||})|^2\rangle$ entering Eq. (A7) as

$$\begin{aligned}\langle|T(\mathbf{k}_{||},\mathbf{k}'_{||})|^2\rangle=&|\langle T(\mathbf{k}_{||},\mathbf{k}_{||})\rangle|^2\delta_{\mathbf{k}_{||}\mathbf{k}'_{||}}+[\langle|T(\mathbf{k}_{||},\mathbf{k}'_{||})|^2\rangle\\&-|\langle T(\mathbf{k}_{||},\mathbf{k}_{||})\rangle|^2\delta_{\mathbf{k}_{||}\mathbf{k}'_{||}}].\end{aligned} \tag{A9}$$

Using this representation and noting that $G_0(\mathbf{k}_{||})$, Eq. (A8), is purely imaginary, Eq. (A7) may be rewritten as follows:

$$\begin{aligned}\langle|G(\mathbf{k}_{\|},\mathbf{k}'_{\|})|^2\rangle=&|G_0(\mathbf{k}_{\|})|^2\{[1-\mathrm{Im}\,G_0^+(\mathbf{k}_{\|})\mathrm{Im}\langle T^+(\mathbf{k}_{\|},\mathbf{k}_{\|})\rangle]^2\\&+|G_0(\mathbf{k}_{\|})|^2[\mathrm{Re}\langle T^+(\mathbf{k}_{\|},\mathbf{k}_{\|})\rangle]^2\}\delta_{\mathbf{k}_{\|},\mathbf{k}'_{\|}}\\&+|G_0(\mathbf{k}_{||})|^2[\langle|T(\mathbf{k}_{||},\mathbf{k}'_{||})|^2\rangle\\&-|\langle T^+(\mathbf{k}_{||},\mathbf{k}_{||})\rangle|^2\delta_{\mathbf{k}_{||}\mathbf{k}'_{||}}]|G_0(\mathbf{k}'_{||})|^2,\end{aligned} \tag{A10}$$

where $\mathrm{Im}\,G_0^+(\mathbf{k}_{||})=-2/\hbar[v_1(\mathbf{k}_{||})+v_2(\mathbf{k}_{||})]$. Comparing the second right-hand terms of Eqs. (A6) and (A10), we obtain (in this non-self-consistent approach) for, the vertex function,

$$W(\mathbf{k}_{||},\mathbf{k}'_{||})=\langle|T(\mathbf{k}_{||},\mathbf{k}'_{||})|^2\rangle-|\langle T^+(\mathbf{k}_{||},\mathbf{k}_{||})\rangle|^2\delta_{\mathbf{k}_{||}\mathbf{k}'_{||}}. \tag{A11}$$

It is easy to see that the flux-conserving transmission amplitude is related to the Green's function through

$$t(\mathbf{k}_{||},\mathbf{k}'_{||})=i\hbar\sqrt{v_2(\mathbf{k}_{||})v_1(\mathbf{k}'_{||})}G^+(\mathbf{k}_{||},\mathbf{k}'_{||}). \tag{A12}$$

For an ideal interface, the transmission amplitude (A12) is diagonal with respect to $\mathbf{k}_{||}$ and defined by Eq. (A8), $t_0(\mathbf{k}_{||},\mathbf{k}_{||})=\sqrt{t_Lt_R}$, where t_L and t_R are defined by Eq. (9).

Thus, according to Eqs. (A10) and (A12) we can define in general the transmission probability as

$$\langle|t(\mathbf{k}_{||},\mathbf{k}'_{||})|^2\rangle=T_0(\mathbf{k}_{||})S_t(\mathbf{k}_{||})\delta_{\mathbf{k}_{||}\mathbf{k}'_{||}}+D_t(\mathbf{k}_{||},\mathbf{k}'_{||}). \tag{A13}$$

Here, $T_0(\mathbf{k}_{||})=t_Lt_R$ is the transmission probability for the ideal interface,

$$\begin{aligned}S_t(\mathbf{k}_{||})=&\left(1+\frac{2}{\hbar[v_1(\mathbf{k}_{||})+v_2(\mathbf{k}_{||})]}\mathrm{Im}\langle T^+(\mathbf{k}_{||},\mathbf{k}_{||})\rangle\right)^2\\&+\frac{4}{\hbar^2[v_1(\mathbf{k}_{||})+v_2(\mathbf{k}_{||})]^2}[\mathrm{Re}\langle T^+(\mathbf{k}_{||},\mathbf{k}_{||})\rangle]^2\end{aligned} \tag{A14}$$

is the specularity factor for transmission at the rough interface, and

$$\begin{aligned}&D_t(\mathbf{k}_{||},\mathbf{k}'_{||})\\&=\frac{16v_2(\mathbf{k}_{||})v_1(\mathbf{k}'_{||})}{\hbar^2[v_1(\mathbf{k}_{||})+v_2(\mathbf{k}_{||})]^2[v_1(\mathbf{k}'_{||})+v_2(\mathbf{k}'_{||})]^2}W(\mathbf{k}_{||},\mathbf{k}'_{||})\end{aligned} \tag{A15}$$

is the diffuse contribution to transmission, where the vertex function $W(\mathbf{k}_{||},\mathbf{k}'_{||})$ is defined by Eq. (A11).

The probability of reflection from the interface may be obtained in a similar manner to the transmission. It is convenient to use the continuity relation at the interface which results in the following relation between the transmission, $t(\mathbf{k}_{||},\mathbf{k}'_{||})$, and reflection, $r(\mathbf{k}_{||},\mathbf{k}'_{||})$, amplitudes:

$$r(\mathbf{k}_{||},\mathbf{k}'_{||})=\sqrt{\frac{v_1(\mathbf{k}_{||})}{v_2(\mathbf{k}_{||})}}t(\mathbf{k}_{||},\mathbf{k}'_{||})-\delta_{\mathbf{k}_{||}\mathbf{k}'_{||}} \tag{A16}$$

or, in terms of the Green's function,

$$r(\mathbf{k}_{||},\mathbf{k}'_{||})=i\hbar\sqrt{v_1(\mathbf{k}_{||})v_1(\mathbf{k}'_{||})}G^{+}(\mathbf{k}_{||},\mathbf{k}'_{||})-\delta_{\mathbf{k}_{||}\mathbf{k}'_{||}}, \tag{A17}$$

which follows from Eq. (A12). Making use of Eqs. (A12) and (A3), we arrive at the following result for the reflection probability:

$$\langle|r(\mathbf{k}_{||},\mathbf{k}'_{||})|^2\rangle=R_0(\mathbf{k}_{||})S_r(\mathbf{k}_{||})\,\delta_{\mathbf{k}_{||}\mathbf{k}'_{||}}+D_r(\mathbf{k}_{||},\mathbf{k}'_{||}), \tag{A18}$$

where $R_0(\mathbf{k}_{||})=|r_L|^2=|r_R|^2$ is the reflection probability for a perfect interface,

$$S_r(\mathbf{k}_{||})=\left[1+\frac{4}{\hbar}\frac{v_1(\mathbf{k}_{||})}{v_1^2(\mathbf{k}_{||})-v_2^2(\mathbf{k}_{||})}\mathrm{Im}\langle T^{+}(\mathbf{k}_{||},\mathbf{k}_{||})\rangle\right]^2 + \frac{16v_1^2(\mathbf{k}_{||})}{\hbar^2[v_1^2(\mathbf{k}_{||})-v_2^2(\mathbf{k}_{||})]^2}[\mathrm{Re}\langle T^{+}(\mathbf{k}_{||},\mathbf{k}_{||})\rangle]^2 \tag{A19}$$

is the specularity factor for reflection, and

$$D_r(\mathbf{k}_{||},\mathbf{k}'_{||})=\frac{16v_1(\mathbf{k}_{||})v_1(\mathbf{k}'_{||})}{\hbar^2[v_1(\mathbf{k}_{||})+v_2(\mathbf{k}_{||})]^2[v_1(\mathbf{k}'_{||})+v_2(\mathbf{k}'_{||})]^2}W(\mathbf{k}_{||},\mathbf{k}'_{||}) \tag{A20}$$

is the diffuse factor for reflection. It is interesting to note from Eqs. (A19) and (9) that random disorder at an interface can result in a specular-reflected beam even when there is no specular beam in the absence of disorder, i.e., when $v_1=v_2$.

The general expressions presented here may serve as a basis for calculation of transmission and reflection probabilities at a rough interface. To do that one needs to use some approximation for the scattering T matrix. Particularly, in order to determine the specularity factors (A14) and (A19) (which are never negative) the average T matrix $\langle T^{+}(\mathbf{k}_{||},\mathbf{k}_{||})\rangle$ should be calculated. The diffuse factors (A15) and (A20) are determined by the vertex function $W(\mathbf{k}_{||},\mathbf{k}'_{||})$, Eq. (A11), which is the variance of $T^{+}(\mathbf{k}_{||},\mathbf{k}'_{||})$ (from its average value).

To the lowest order of perturbation theory in the impurity potential $V_i(\mathbf{r})=V_i(\rho)\,\delta(z)$ with the properties given by Eqs. (14) and (15) the general results of this appendix reduce to the expressions given in the text of the paper. For example, in this approximation Eq. (A3) for the average Green's function $\langle G(z,z';\mathbf{k}_{||},\mathbf{k}_{||})\rangle$ coincides with Eq. (20).

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