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Exchange coupling in magnetic multilayers: effect of partial confinement of carriers

J Mathon†, Murielle Villeret† and D M Edwards‡

† Department of Mathematics, City University, London EC1V 0HB, UK
‡ Department of Mathematics, Imperial College of Science, Technology and Medicine, London SW7 2BZ, UK

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Abstract. The exchange coupling $J(\ell)$ between magnetic layers across a non-magnetic spacer is observed to oscillate as a function of the spacer thickness ℓ. In an earlier work a theory of the oscillatory exchange was proposed which shows that the oscillation periods are characteristic of the spacer. The theory relied on the assumption of an infinitely large exchange splitting in the magnetic layers, which leads to complete confinement of magnetic carriers of one spin in the ferromagnetic configuration of the sandwich. While this may be valid for strong ferromagnets such as Co or Ni, the complete confinement model is not a realistic approximation for iron which has holes in its majority-spin band. The theory is now generalized to the case of partial confinement of carriers in the spacer appropriate to a sandwich with weakly ferromagnetic layers. An exactly solvable hole-gas model of the coupling as well as numerical tight-binding results are presented which demonstrate that the oscillation period is unaffected but the amplitude and phase depend critically on the degree of confinement. Asymptotic expansions for $J(\ell)$ valid at finite temperature and for an arbitrary single tight-binding band are also obtained. They show that the period and temperature dependence of the oscillations are directly related to the properties of the spacer Fermi surface but the amplitude and phase depend also on the exchange splitting in the ferromagnetic layers.

1. Introduction

During the last few years, much attention has been paid to the properties of layered structures consisting of alternating magnetic and non-magnetic materials. The most commonly studied magnetic multilayers are those consisting of a ferromagnetic transition metal such as iron, cobalt or nickel and a non-magnetic transition or noble metal. The growth of such materials, with interfaces sharp on an atomic scale, has been made possible by recent advances in molecular beam epitaxy (MBE) and sputtering techniques. The study of layered structures such as Fe/Cr, Co/Cr, Co/Cu or Co/Ru, is not only of fundamental interest but holds promise of potential applications in magnetic storage technology.

It was discovered experimentally [1–6] that the magnetic moments of neighbouring magnetic layers are aligned parallel or antiparallel depending on the thickness of the intervening non-magnetic spacer layer. This implies an exchange coupling between the magnetic layers which oscillates as a function of spacer thickness. The period of oscillations in multilayers with noble and transition metal spacers can be as large as 10–20 Å. It is also found [7] that the strength of the exchange coupling increases

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systematically with increasing number of d electrons in the spacer and decreases from 3d to 4d to 5d metals. The oscillation periods observed in noble metal superlattices can be interpreted in terms of RKKY coupling [8–10]. However, an explanation of the physical mechanism responsible for the oscillations through a transition metal spacer is needed.

A specific model for the exchange coupling through a non-magnetic transition metal spacer has been developed by Edwards *et al* [11, 12] for a sandwich consisting of two semi-infinite transition metal ferromagnets separated by a spacer containing N atomic planes. The original model is based on several simplifying assumptions:

(i) The exchange coupling is dominated by the d band and hybridization with the sp conduction band is omitted.

(ii) Interactions between electrons in the non-magnetic spacer are neglected.

(iii) The width of the d band is the same in the magnetic and non-magnetic metals.

(iv) The number of minority-spin electrons per atom in the ferromagnet is the same as the number of electrons per atom of either spin in the non-magnetic spacer.

(v) The d band for majority carriers is full, i.e. the magnetic metal is a strong ferromagnet.

(vi) The five-orbital d band is replaced by a single tight-binding s band.

Assumptions (i)–(iv) are quite reasonable for a system such as Fe/Cr. It is, therefore, most important to relax assumptions (v) and (vi). The condition (v) is combined, in [11] and [12], with an additional assumption of an infinitely large exchange splitting in the magnetic metal. This leads to complete confinement of carriers of one spin in the spacer layer in the ferromagnetic configuration of the sandwich. The exchange potentials, which are equivalent in this model to two infinitely high potential barriers, thus lead to size quantization in the direction perpendicular to the sandwich. The dependence of the exchange coupling on the thickness of the spacer can then be obtained using a formal analogy with the de Haas–van Alphen effect. In the dHvA effect the magnetization oscillates as a function of an applied magnetic field and the oscillations occur because electron energy levels quantized in the field pass through the Fermi level as the strength of the field is increased. Similarly, size-quantized levels crossing the Fermi level as the spacer thickness is varied cause oscillations in the interlayer exchange coupling [13]. An important feature of this approach is that the period and amplitude of the oscillations are linked to the size and shape of the Fermi surface of carriers in the spacer layer. In particular, it is found that the period of the oscillations depends on the position of the Fermi level in the band and becomes very long when the Fermi surface approaches the zone boundary.

A theoretical study [14] of the Fe/Cr system, using a canonical five-orbital d band but still retaining the assumption of completely confined carriers shows that the exchange coupling exhibits oscillations with components of different periods in agreement with experiment [2–6]. However, the calculated exchange coupling has a much larger amplitude than observed and has the wrong phase. It was argued that this discrepancy can be attributed to the assumption of complete carrier confinement which is unrealistic for iron.

The purpose of this paper is to extend and generalize the preliminary results of [14] for the case of partial confinement of carriers in the spacer, thereby relaxing the assumption of a full majority spin band (assumption (v)). This should give a

better description of a weak ferromagnet such as Fe. Even for a strong ferromagnet like Co, hybridization of the d band with the sp conduction band is expected to introduce effects similar to partial confinement. In the partial confinement model we no longer have size quantization of the carriers. This precludes direct application of the theory developed in [11] and [12]. For partially confined carriers, the size-quantized levels are replaced by resonances and we have to modify the theory accordingly. In section 2, we give a general formulation of the partial confinement model. The actual evaluation of the exchange coupling depends on the band structure chosen to describe the sandwich and is discussed in sections 3 and 4 for two different models. In section 3, a hole-gas model is used to determine the exchange coupling analytically for an arbitrary exchange splitting in the ferromagnetic layers. This is achieved through a generalization of an asymptotic expansion obtained in [11,12]. In section 4 the asymptotic expansion, applicable to partially confined carriers, is extended to an arbitrary tight-binding band. The exchange coupling is also investigated numerically. It is found, for both hole-gas and tight-binding models, that, notwithstanding the absence of size quantization, the period and temperature dependence of the oscillations are still directly related to the properties of the Fermi surface in the spacer. However, the amplitude and phase now depend strongly on the exchange splitting in the ferromagnetic layers.

2. Partial confinement model

In [11] and [12] we carried out a comprehensive investigation of the interlayer exchange coupling $J(\ell)$ for a single-orbital tight-binding band structure of the spacer layer using the complete confinement model. As discussed in [11], even this simplest model exhibits many of the observed features of the oscillatory exchange coupling. We have generalized [14] this work to a canonical five-orbital d band which allowed us to calculate the exchange coupling for a (100) Fe/Cr/Fe sandwich. This numerical calculation retaining the assumption of complete confinement leads to an oscillatory exchange which has short- and long-period components, as observed [4], but the calculated oscillation amplitude is much too large and has the wrong phase. Clearly, the assumption of complete confinement is not realistic for Fe/Cr since iron, unlike nickel or cobalt, does have holes in the bulk majority-spin band. It is therefore necessary to extend the theory to the case of partially confined carriers.

Although, in principle, we can calculate numerically the interlayer exchange coupling $J(\ell)$ for a multi-orbital band structure [14], the computational effort is so large that no systematic study of the effect of partial confinement using this brute force approach is possible at this stage. We shall, therefore, first investigate in section 3 the effect of partial confinement for a hole-gas model and then extend the treatment to a single tight-binding band in section 4. The formulation of the partial confinement model is common to both cases and is described in this section.

We use a generalized Hubbard Hamiltonian [11] with parameters chosen to approximate the situation in an Fe/Cr/Fe sandwich with two semi-infinite iron layers separated by a chromium layer of thickness ℓ. Since iron has about 4.8 and 2.6 d electrons per atom in the majority- and minority-spin bands, respectively, and paramagnetic chromium has about 2.7 electrons per atom in each spin band there is an almost exact match between the chromium d band and minority iron d band. We wish to retain this important feature of the Fe/Cr system in our model. We shall,

therefore, assume that holes moving from the minority band of the ferromagnetic layers to the non-magnetic layer experience no change in their local potential, which is taken to be zero. On the other hand, holes moving from the non-magnetic layer to the majority band in the ferromagnetic layers experience a potential step equal to the bulk exchange splitting V in the ferromagnet. To avoid confusion, we adopt the following convention for the spin orientation. The total electron spin moment of the left ferromagnet is always assumed to point up. The up-spin orientation ($\uparrow$) of holes moving across the sandwich is defined as that of holes in the minority-spin band of the left ferromagnet, the down-spin orientation ($\downarrow$) is that of holes in the majority-spin band.

Using this convention, we can easily visualize the local potentials V^{σ} seen by holes of spin σ in the ferromagnetic and antiferromagnetic configurations of the sandwich. They are shown schematically in figure 1.

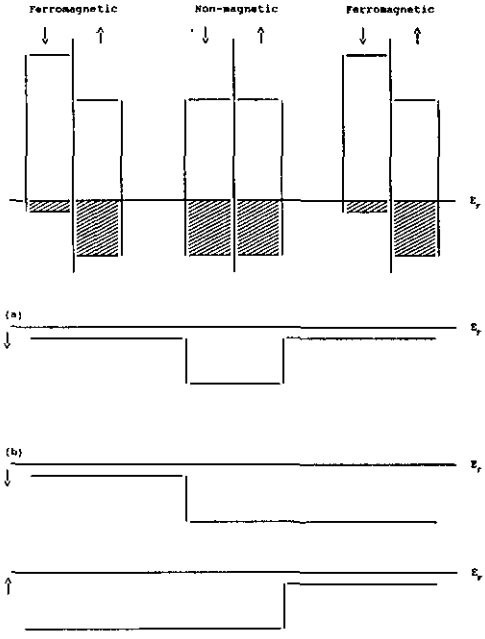

Figure 1. Schematic representation of the majority- and minority-spin bands of the magnetic and non-magnetic layers of the sandwich in its ferromagnetic configuration. The shaded areas show the regions of the bands that are occupied by holes up to the Fermi level E_F common to the whole sandwich. In (a) we show the potential well experienced by holes in the majority-spin band ($\downarrow$-spin holes) in the ferromagnetic configuration of the system. The up-spin holes moving from the minority band of the ferromagnetic layers to the non-magnetic layers experience no change in their local potential which is taken to be zero. In (b) we show the potentials experienced by $\downarrow$- and $\uparrow$-spin holes in the antiferromagnetic configuration of the sandwich. The schematic representation of the bands in this case is not shown here. It is obtained from that in the ferromagnetic configuration by interchanging the majority and minority bands of the right ferromagnet.

It is clear that there are two parameters in our model. The exchange splitting V determines the magnetization in the bulk of the ferromagnetic layers and the Fermi

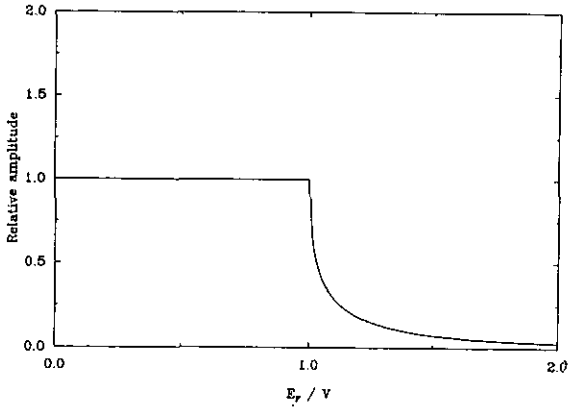

Figure 2. Relative amplitude of the exchange coupling $J(\ell)$ as a function of E_F/V taken from the asymptotic formulae (3.9) and (3.10) for the hole-gas model.

level E_F, common to the whole sandwich, determines the number of holes per atom in the sandwich. Although E_F and V could be chosen to mimic the Fe/Cr system, we cannot expect quantitatively correct results with a model in which the d bands in Fe/Cr are approximated either by parabolic or single tight-binding bands. We shall, therefore, treat E_F and V as adjustable parameters and investigate the general effect of partial confinement ($V < E_F$) on the exchange coupling. This means that we are going to discuss the dependence of the interlayer exchange coupling on the exchange splitting V in the ferromagnetic layers.

The interlayer exchange coupling $J(\ell)$ is defined as the difference between the total energies of the ferromagnetic and antiferromagnetic configurations of the magnetic layers per unit area of the sandwich. It was shown in [11] that $J(\ell)$ for the complete confinement model is given by

$$J(\ell) = [\Omega(\ell) - \Omega(\infty)]/A \tag{2.1}$$

where $\Omega(\ell)$ is the thermodynamic potential of $\downarrow$-spin holes in the ferromagnetic configuration of the sandwich and A is the surface area. The thermodynamic potential $\Omega(\ell)$ is defined by

$$\Omega(\ell) = E(\ell) - E_F n(\ell) \tag{2.2}$$

where $E(\ell)$ is the total energy and $n(\ell)$ the total number of $\downarrow$-spin holes confined in the spacer layer in the ferromagnetic configuration. We recall that both $E(\ell)$ and $n(\ell)$ are measured relative to a reference state with a constant bulk density of holes, i.e. $\Omega(\ell) = \Omega_{tot}(\ell) - \Omega_{ref}(\ell)$, where $\Omega_{tot}(\ell)$ and $\Omega_{ref}(\ell)$ are the total and reference thermodynamic potentials, respectively. It follows that $\Omega(\ell)$ for our infinite sandwich remains finite since deviations from the bulk reference state occur only in the vicinity of the two interfaces.

We may use the same expression (2.1) for $J(\ell)$ in the partial confinement case but the reference state now needs to be modified since we have holes with different densities in the non-magnetic and magnetic layers. In the non-magnetic layer the reference state is that of holes with a constant bulk density appropriate to Fermi

energy E_F and potential $V^{\downarrow} = 0$. In the magnetic layers we take as a reference the state of bulk holes with a lower density appropriate to the same E_F but a finite potential $V^{\downarrow} = V$ (in the case of the tight-binding model V is the local potential in each atomic plane). Although this method of calculating $J(\ell)$ is not a fully self-consistent treatment of a generalized Hubbard model, as it is in the complete confinement case, it is expected to yield reliable results.

The calculation of the exchange coupling $J(\ell)$ requires the evaluation of $\Omega(\ell)$ for partially confined $\downarrow$-spin holes in the ferromagnetic configuration. This involves a summation over all one-particle energies of holes moving in the presence of a square-well potential. In the complete confinement case the hole energies were size-quantized in an infinitely deep well and we performed the summation over the discrete energies directly by means of the Poisson summation formula. This is no longer possible for partially confined holes since we have to include the contribution of the continuous spectrum above the top of the well. We shall, therefore, express the total thermodynamic potential Ω_{tot} in terms of the density of states $\mathcal{D}(E, \ell)$. The thermodynamic potential Ω_{tot}, at finite temperature T, is then given by

$$\Omega_{tot} = -k_B T \int_{-\infty}^{\infty} \ln\{1 + \exp[(\mu - E)/k_B T]\}\mathcal{D}(E, \ell)\,dE \tag{2.3}$$

where μ is the chemical potential and the argument ℓ in $\mathcal{D}(E, \ell)$ indicates that the density of states is a function of the width of the potential well. For the gas model, $\mathcal{D}(E, \ell)$ is clearly the total density of states for the whole sandwich. In the case of a tight-binding band it is the sum of all the local densities of states in each atomic plane of the sandwich.

The actual evaluation of Ω_{tot} depends on the band structure chosen to describe the sandwich. In the next section we treat the case of a gas model which is solvable analytically.

3. Effect of partial confinement of magnetic carriers for a hole gas model

We first consider a hole-gas model of the exchange coupling between two ferromagnetic layers to illustrate how our theory based on complete confinement of magnetic carriers in the spacer layer can be generalized to partially confined carriers. A special feature of the gas model is that the thickness ℓ of the spacer is a continuous variable, which allows us to differentiate Ω_{tot} with respect to ℓ. It will be seen that a significant simplification achieved in calculating $d\Omega_{tot}/d\ell$ is that we only require the value of the local density of states at the edge of the well $z = \ell$ rather than the total density of states. The exchange coupling $J(\ell)$ is then simply obtained by integrating with respect to ℓ. This method was already used to derive equation (3.5) of [14] which gives the exchange coupling for a sandwich in which the magnetic layers remain strong ferromagnets but with finite exchange splitting.

Using this approach, we need to determine the derivative with respect to ℓ of the total density of states $d\mathcal{D}(E, \ell)/d\ell$. It is shown in the appendix that it is given by

$$\frac{d\mathcal{D}(E, \ell)}{d\ell} = -\frac{V}{\pi}\frac{d}{dE}\,\mathrm{Im}\sum_{k_\parallel} G(\ell, \ell, E, k_\parallel). \tag{3.1}$$

Here, $G(\ell, \ell, E, k_\parallel)$ is the local one-electron Green function in a mixed representation which is taken to be the position representation in the direction

z perpendicular to the layers and the momentum representation in the direction parallel to the layers. The summation in equation (3.1) is over the two-dimensional wave vector $\boldsymbol{k}_{\parallel}$ parallel to the layers. Differentiating equation (2.3) with respect to ℓ, substituting for $\mathrm{d}\mathcal{D}(E,\ell)/\mathrm{d}\ell$ from equation (3.1) and integrating by parts the energy integral in equation (2.3), we obtain

$$\frac{\mathrm{d}\Omega_{\mathrm{tot}}}{\mathrm{d}\ell} = \frac{V}{\pi}\sum_{\boldsymbol{k}_{\parallel}}\int_{-\infty}^{\infty}\frac{\operatorname{Im} G(\ell,\ell,E,\boldsymbol{k}_{\parallel})}{1+\exp[(E-\mu)/k_{\mathrm{B}}T]}\,\mathrm{d}E. \tag{3.2}$$

It is straightforward to calculate analytically $G(\ell,\ell,E,\boldsymbol{k}_{\parallel})$ for energies both inside and outside the well and we can, therefore, evaluate $\mathrm{d}\Omega_{\mathrm{tot}}/\mathrm{d}\ell$ from equation (3.2) numerically. The corresponding numerical results will be discussed later. However, it is far more illuminating to have an asymptotic expansion for $J(\ell)$ valid for large ℓ, similar to the asymptotic formula obtained in [11] in the complete confinement model. Our derivation of such an asymptotic formula is based on an observation that in the complete confinement model oscillations in $J(\ell)$ arise because size-quantized energy levels of holes confined in the spacer pass across the Fermi level E_{F} as the thickness ℓ varies. For partially confined holes, E_{F} lies above the top of the well and instead of size-quantized levels we now have resonances crossing the Fermi level. Since the resonances have evolved continuously from bound states when E_{F} is below the top of the well, it is natural to expect that the resonances at E_{F} control oscillations in $J(\ell)$ for partially confined holes.

To formalize the argument we need to examine the Green function at energies $E > V$. It is straightforward to show that $\operatorname{Im} G(\ell,\ell,E,\boldsymbol{k}_{\parallel})$ is given by

$$\operatorname{Im} G(\ell,\ell,E,\boldsymbol{k}_{\parallel}) = -[2m(E-E_{\parallel}-V)/\hbar^2]^{1/2} \times \frac{2(E-E_{\parallel})-V\sin^2(\beta\ell)}{4(E-E_{\parallel})(E-E_{\parallel}-V)+V^2\sin^2(\beta\ell)} \tag{3.3}$$

where $\beta = [2m(E-E_{\parallel})/\hbar^2]^{1/2}$ and $E_{\parallel} = \hbar^2 k_{\parallel}^2/2m$. As anticipated, we find that $\operatorname{Im} G$ is an even periodic function of ℓ with period π/β. This corresponds to resonant peaks in the density of states passing through a given energy as ℓ is varied and the energy dependence of the period is the same as that for energies inside the well. We can, therefore, expand $\operatorname{Im} G$ into a cosine Fourier series. Equation (3.2) then takes the form

$$\frac{\mathrm{d}\Omega_{\mathrm{tot}}}{\mathrm{d}\ell} = \frac{VA}{4\pi^3}\int\int \mathrm{d}\boldsymbol{k}_{\parallel} \times \int_{-\infty}^{\infty}\frac{\{a_0(E,\boldsymbol{k}_{\parallel}) + \operatorname{Re}\sum_{s=1}^{\infty} a_s(E,\boldsymbol{k}_{\parallel})\exp[2is\ell\beta(E,\boldsymbol{k}_{\parallel})]\}}{1+\exp[(E-\mu)/k_{\mathrm{B}}T]}\,\mathrm{d}E \tag{3.4}$$

where $a_s(E,\boldsymbol{k}_{\parallel})$ is the Fourier component of $\operatorname{Im} G$.

It can be seen that $\mathrm{d}\Omega_{\mathrm{tot}}/\mathrm{d}\ell$ contains both non-oscillatory and oscillatory components. The non-oscillatory component coming from $a_0(E,\boldsymbol{k}_{\parallel})$ can be readily recognized as the derivative with respect to ℓ of the reference term $\Omega_{\mathrm{ref}}(\ell)$. Since this constant term should be subtracted from $\mathrm{d}\Omega_{\mathrm{tot}}/\mathrm{d}\ell$, the exchange coupling $J(\ell)$ is determined entirely by the oscillatory term in equation (3.4).

For large ℓ, the imaginary exponential in equation (3.4) oscillates rapidly as a function of $k_\parallel$ and the dominant contribution to the integral with respect to $k_\parallel$ comes only from the vicinity of points at which β reaches an extremum as a function of $k_\parallel$. We can therefore evaluate this integral using the method of stationary phase. Since the amplitudes $a_s(E,k_\parallel)$ are slowly varying functions of $k_\parallel$, we approximate them by $a_s(E,k_\parallel) \simeq a_s(E,k_\parallel^0)$, where $k_\parallel^0$ is an extremal point. We can then expand β in the argument of the exponential function up to the second order around the extremal point $k_\parallel^0$ and evaluate the resultant $k_\parallel$ integral analytically using the method already described in [11]. This yields

$$\frac{d\Omega}{d\ell} = \frac{VA}{4\pi^2}\,\mathrm{Re}\sum_s \frac{\sigma}{\ell s}\int_{-\infty}^{\infty} a_s(E,k_\parallel^0)\left|\frac{\partial^2\beta}{\partial k_x^2}\frac{\partial^2\beta}{\partial k_y^2}\right|^{-1/2}\frac{\exp[2is\ell\beta(E,k_\parallel^0)]}{1+\exp[(E-\mu)/k_BT]}\,dE \tag{3.5}$$

where the second derivatives are taken at the extremal point $k_\parallel^0$ and the factor σ takes the value i for a minimum, $-$i for a maximum and 1 for a saddle point. We recall that we have dropped the non-oscillatory reference term and this is the reason why, in equation (3.5), we write Ω rather than Ω_{tot}.

It remains to perform the energy integral in equation (3.5). The integrand contains the product of two rapidly varying functions of the energy, i.e., the Fermi function and the factor $\exp[2is\ell\beta(E,k_\parallel^0)]$. The region in which the Fermi function is essentially constant does not contribute to the integral because of rapid oscillations of the function $\exp[2is\ell\beta(E,k_\parallel^0)]$. The only significant contribution comes from a narrow interval around the Fermi surface where the Fermi function varies rapidly. This argument is valid not only for energies $E > V$ but also in the case of bound states in the well ($E < V$) which is discussed in [11] (see also the appendix). We can apply it to the integral in equation (3.5) over the whole energy range provided there is no discontinuity in Im G across the well at $E = V$. In fact, we can imagine that the energy integral is taken in a complex plane over a line displaced infinitesimally above the real axis. The Green function is an analytic function off the real axis and, therefore, a continuous function of the complex energy $E + i\eta$, where η is a positive infinitesimal quantity. It follows that oscillations of Im G for E in the well join smoothly with the oscillations for E above the well and we can evaluate the energy integral in equation (3.5) by considering only the contribution from the vicinity of the Fermi surface, as discussed above. The evaluation of the energy integral using this approximation is described in [11] and it is quite straightforward to show that the relevant oscillatory term $d\Omega/d\ell$ is given by

$$\frac{d\Omega}{d\ell} = -\frac{VAk_BT}{4\pi\ell}\sum_s \mathrm{Re}\,\frac{i\sigma}{s}\frac{a_s(\mu,k_\parallel^0)}{\sinh[2\ell s\pi(\partial\beta/\partial E)k_BT]} \times\left|\frac{\partial^2\beta}{\partial k_x^2}\frac{\partial^2\beta}{\partial k_y^2}\right|^{-1/2}\exp[2is\ell\beta(\mu,k_\parallel^0)]. \tag{3.6}$$

The exchange coupling $J(\ell)$ defined by equation (2.1) can now be obtained by integration of equation (3.6) with respect to ℓ. This yields

$$J(\ell) = -\frac{Vk_BT}{8\pi\ell\beta(\mu,k_\parallel^0)}\sum_s \mathrm{Re}\,\frac{\sigma}{s^2}\frac{a_s(\mu,k_\parallel^0)}{\sinh[2\ell s\pi(\partial\beta/\partial E)k_BT]}$$

$$\times \left| \frac{\partial^2 \beta}{\partial k_x^2} \frac{\partial^2 \beta}{\partial k_y^2} \right|^{-1/2} \exp[2is\ell\beta(\mu, k_\parallel^0)] \tag{3.7}$$

where we have kept only the leading term of order $1/\ell^2$ and all the derivatives are evaluated at the stationary point and for $E = \mu$. Naturally, the contributions of all the stationary points of β need to be included in equation (3.7).

As in the complete confinement model discussed in [11], we find that $J(\ell)$ oscillates as a function of ℓ with a period $\pi/\beta(\mu, k_\parallel^0)$ which is determined by the extremal radius of the Fermi surface in the spacer layer, the oscillation amplitude decreases with ℓ as $1/\ell^2$ (at $T = 0$) and the temperature dependence of the coupling is again governed by the velocity of carriers at the extremal points at the Fermi surface.

However, an entirely new feature for partially confined carriers is the presence of the Fourier component $a_s(\mu, k_\parallel^0)$ evaluated at the extremal points of the spacer-layer Fermi surface. The overall amplitude of oscillations in the exchange coupling is, therefore, controlled by the product of two factors: the curvature of the Fermi surface in the non-magnetic spacer layer and the Fourier component of the imaginary part of the one-electron Green function taken at the edge of the spacer layer. The latter factor, which is absent in the complete confinement model, reflects the magnitude of the exchange splitting in the ferromagnetic layers and will be shown to have a dramatic effect on the overall strength of the exchange coupling.

For the parabolic band considered here, we have only one extremum (minimum) at $k_\parallel = 0$ and $\partial\beta/\partial E = m/(\hbar^2\beta)$, $\partial^2\beta/\partial k_x^2 = 1/k_F$ hold at the extremum (we take the sandwich to be parallel to the x–y plane). The Fourier component of $\operatorname{Im} G(\ell, \ell, E_F, 0)$ obtained from equation (3.3) is given by

$$a_s(E_F, k_\parallel^0) = -2\frac{k_F}{V^{2s+1}}[8E_F(E_F - V) + V^2 - 4\sqrt{E_F(E_F - V)}(2E_F - V)]^s. \tag{3.8}$$

At zero temperature, the asymptotic formula for $J(\ell)$ valid for $E_F > V$ takes a very simple form

$$J(\ell) = (E_F/4\pi^2\ell^2)\sum_s (s^3V^{2s})^{-1}[8E_F(E_F - V) + V^2 - 4(E_F(E_F - V))^{1/2}(2E_F - V)]^s \sin(2sk_F\ell). \tag{3.9}$$

To pinpoint the differences between the models with completely and partially confined holes, we also reproduce here an asymptotic formula for holes confined to a finite well ($E_F < V$). It was given in [14] and a detailed derivation is presented in the appendix. The result is

$$J(\ell) = \frac{E_F}{4\pi^2\ell^2}\sum_{s=1}^{\infty}\frac{1}{s^3}\sin 2s(k_F\ell + \psi(E_F)) \tag{3.10}$$

where the phase ψ is a function of energy defined by

$$\tan\psi(E) = 2\sqrt{E(V - E)}/(V - 2E). \tag{3.11}$$

Let us discuss first the case of confined holes, i.e. the case when the magnetic layers in a sandwich are strong ferromagnets such as cobalt or nickel. It can be

seen from equation (3.10) that for a fixed E_F the amplitude of oscillations in the exchange coupling remains constant as a function of the exchange splitting V as long as V is greater than E_F but there is a phase shift ψ defined by equation (3.11). Thus the only effect of varying E_F/V continuously from 0 to 1 is that the phase of the principal term $\sin(2k_F\ell + 2\psi)$ shifts continuously from 0 to 2π. We recall that the complete confinement model used in [11] corresponds to the limit of an infinite exchange splitting and is thus just a special case of equation (3.10) obtained for $E_F/V \to 0$.

Consider now the case of partially confined holes with $E_F > V$ corresponding to magnetic layers which are weak ferromagnets such as iron. It can be seen from equation (3.9) that the phase locks at $\psi = 0$ for all values of $(E_F/V) > 1$ but the relative amplitude of oscillations in the exchange coupling decreases dramatically with increasing E_F/V . This is illustrated in figure 2. We note that both the amplitude and phase are continuous at $(E_F/V) = 1$ where the crossover from complete to partial confinement takes place.

It is interesting to assess the accuracy of the asymptotic expansions (3.9) and (3.10), which are valid to order $O(1/\ell^2)$, by comparing them with numerical results obtained from equation (3.2) at $T = 0$K. We shall make the actual comparison for the derivative of the exchange coupling $d\Omega/d\ell$ since only this quantity can be easily determined numerically from equation (3.2). The numerical results for $d\Omega/d\ell$ plotted as a function of the spacer layer thickness ℓ are shown in figure 3 for $E_F/V = 0.005$ (*complete confinement*) and $E_F/V = 1.25$ (*partial confinement*). The corresponding asymptotic results are displayed in figure 4.

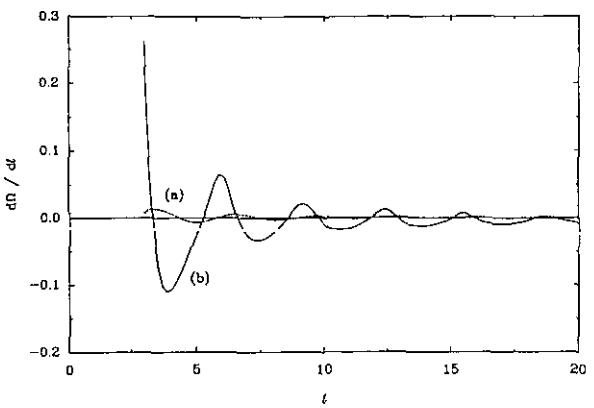

Figure 3. Derivative of the thermodynamic potential, $d\Omega/d\ell$, as a function of spacer thickness ℓ obtained numerically from equation (3.2) at $T = 0$K for partial (*a*) and complete (b) confinement of magnetic carriers: (a) $E_F/V = 1.25$ (dashed curve); (*b*) $E_F/V = 0.005$ (*solid curve*). $d\Omega/d\ell$ *is expressed in units of the Fermi energy* E_F *and* all lengths are given in units of $1/k_F$.

Although there is very good agreement between the amplitudes and periods of oscillations for the two sets of results in figures 3 and 4, there appears an initial phase shift between the asymptotic and numerical results. This is a consequence of limiting the asymptotic expansion to the leading term which is of order $1/\ell^2$. It is shown in the appendix that when the asymptotic expansion is extended to include

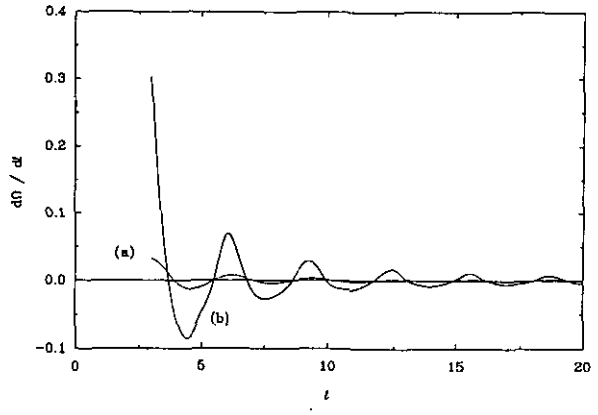

Figure 4. Asymptotic behaviour of $d\Omega/d\ell$ at $T = 0$ K as a function of spacer thickness ℓ for partially (*a*) and completely (*b*) confined holes. Units of energy and length as in figure 3. Same parameters as in figure 3.

terms in $1/\ell^3$ this apparent phase shift disappears. However, there remains a real phase shift between oscillations in the exchange coupling for the complete and partial confinement models as demonstrated in figure 3. We shall return to this interesting question in section 4 where our theory is extended to more realistic tight-binding bands.

4. Effect of partial confinement of magnetic carriers for a tight-binding model

We now apply the model of Sec.2 to a sandwich with a single-orbital tight-binding band structure. As in [11], we shall investigate the exchange coupling between two semi-infinite ferromagnets separated by a non-magnetic layer of N atomic planes using the Hubbard Hamiltonian

$$H = \sum_{i,j,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \sum_{i} U_i n_{i\uparrow} n_{i\downarrow} \tag{4.1}$$

where $c^{\dagger}_{i\sigma}$ creates a hole of spin σ on site i and $n_{i\sigma} = c^{\dagger}_{i\sigma} c_{i\sigma}$. We assume the hopping parameters t_{ij} are the same in the magnetic and non-magnetic metals and $U_i = U_0$ for sites i in the ferromagnetic layers and $U_i = 0$ in the spacer layer. It follows that we again have two parameters in our model: the intra-atomic Coulomb interaction U_0 determines the exchange splitting V in the bulk of the ferromagnetic layers and the common Fermi level E_F determines the number of holes per atom in the sandwich. Throughout this section we measure all the energies in units of $W/6$, where W is the band width.

We may use equation (2.1) for the exchange coupling $J(\ell)$ and equation (2.3) for the thermodynamic potential $\Omega(\ell)$ bearing in mind that $\mathcal{D}(E, \ell)$ is the total density of states for down-spin holes in the ferromagnetic configuration of a sandwich described by the tight-binding Hamiltonian (4.1). However, since $\ell = Na$ is now discrete (a is the separation between two neighbouring atomic planes in the spacer layer), we can no longer differentiate $\Omega_{tot}(\ell)$ with respect to ℓ but have to calculate Ω_{tot} directly from equation (2.3). Expressing the density of states in terms of the imaginary

part of the local Green function $G_{nn}(E, k_\parallel, N)$ in the mixed position-momentum representation, we obtain

$$\Omega_{tot}(N) = (k_B T/\pi) \sum_{k_\parallel} \int_{-\infty}^{\infty} \ln\{1 + \exp[(\mu - E)/k_B T]\} \times \mathrm{Im} \sum_n G_{nn}(E, k_\parallel, N)\, \mathrm{d}E \tag{4.2}$$

where n labels atomic planes parallel to the sandwich and the summation over $k_\parallel$ is over the two-dimensional wave vectors in the first Brillouin zone.

The calculation of Ω_{tot} from equation (4.2) requires the local Green function $G_{nn}(E, k_\parallel, N)$ in each atomic plane of the sandwich. However, since we are only interested in the change of Ω_{tot} relative to the reference Ω_{ref}, it is sufficient to calculate the local G_{nn} for the N atomic planes of the spacer and a finite number M of adjacent ferromagnetic planes on each side. For sufficiently large M, $\Omega(N)$ becomes essentially independent of M and we find that this occurs for M in the range 5 to 10.

As in section 3, we now have two options. We may determine Ω_{tot} from equation (4.2) numerically or use an asymptotic expansion to evaluate the summation over $k_\parallel$ and the energy integral approximately. In either case, we first need to calculate the local Green function $G_{nn}(E, k_\parallel, N)$. For a tight-binding model, this can no longer be done analytically and the most convenient way to determine $G_{nn}(E, k_\parallel, N)$ for a stack of $N + 2M$ atomic planes sandwiched between two semi-infinite substrates is to use the method of adlayers [15]. Since the method of adlayers starts from the surface Green function for a semi-infinite substrate which is known analytically [16], the local G_{nn} is obtained with machine accuracy and no numerical error is introduced at this stage.

We first describe the numerical evaluation of Ω_{tot} at zero temperature for a simple cubic lattice and (100) orientation of the layers. It is convenient to convert the summation over $k_\parallel$ in equation (4.2) into an integral introducing a two-dimensional density of states $\mathcal{D}_{2d}(E_\parallel)$ which yields

$$\Omega_{tot} = -(1/\pi) \int_{-2}^{2} \mathrm{d}E_\parallel \mathcal{D}_{2d}(E_\parallel) \int_{-\infty}^{E_F} (E - E_F)\, \mathrm{Im} \sum_n G_{nn}(E, E_\parallel, N)\, \mathrm{d}E. \tag{4.3}$$

The integration over E requires a large number of energy points since $\mathrm{Im}\, G(E, E_\parallel, N)$ has poles on the real axis. In order to gain speed and accuracy, we perform this integration in the complex plane using a method described in [17]. However, even with this extremely efficient integration method, the evaluation of Ω to the required accuracy takes many hours of computer time.

A significant simplication can be obtained for Fermi energies $-3 \leqslant E_F \leqslant -1$ for which it is a reasonable approximation to use a constant $\mathcal{D}_{2d}(E_\parallel)$. We take it equal to $\frac{1}{4}$ for $|E_\parallel| \leqslant 2$ and zero otherwise (we recall that we express all energies in units of W/6). Using this approximation, integrating by parts in equation (4.3), and noting that $\sum_n G_{nn}(E, E_\parallel, N)$ is a function of the single variable $E - E_\parallel$, we can reduce equation (4.3) to a single energy integral

$$\Omega(N) = (1/8\pi) \int_{-\infty}^{E_F} (E - E_F)^2$$

$$\times \operatorname{Im} \sum_n [G_{nn}(E+2, N) - G_{nn}(E-2, N)]\, \mathrm{d}E. \tag{4.4}$$

This is evaluated numerically using again a complex contour integration and we obtain $J(N)$, given by equation (2.1), by subtracting the appropriate reference contribution as described in [14]. The results for complete ($E_F/V = 0.005$) and partial ($E_F/V = 1.25$) confinements are displayed in figure 5. In both cases $E_F = 0.5$, measured from the bottom of the spacer band, was chosen to reproduce rapid two monolayer oscillations observed in Fe/Cr.

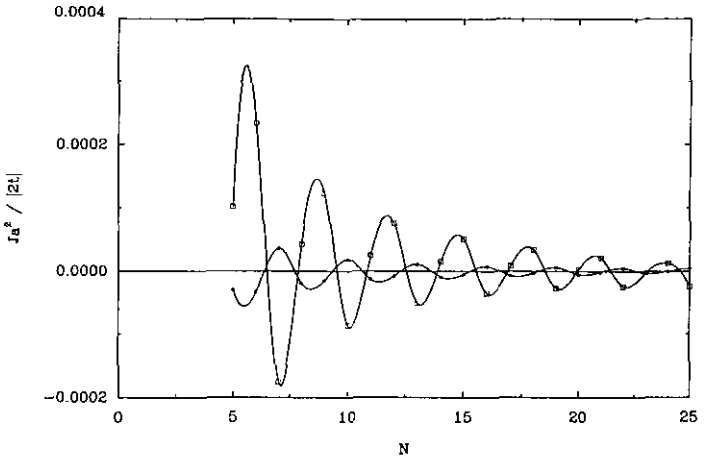

Figure 5. Comparison of the amplitudes and phases of oscillations in the exchange coupling J obtained numerically from equation (4.4) for a simple cubic tight-binding model. J is plotted as a function of the number N of atomic planes in the spacer layer for completely and partially confined carriers. The squares correspond to the case where the Fermi level lies above the well ($E_F/V = 1.25$) whereas the circles are for a Fermi level lying inside the confining potential ($E_F/V = 0.005$). $E_F = 0.5$ measured from the bottom of the spacer band and J is given in units of $2|t| = W/6$, where W is the band width.

As for the hole-gas model, the most important feature is the dramatic reduction of the amplitude which occurs in going from complete to partial confinement. Such a large reduction is quite remarkable considering that the number of holes we have introduced in the majority-spin band is quite small ($n_\uparrow/n_\downarrow \simeq 0.09$). There is also a phase shift of almost exactly π between the two curves in figure 5. We recall that in the hole-gas model the corresponding phase shift was somewhat smaller indicating that it is a model dependent quantity.

In the approximation of a constant two-dimensional density of states we are restricted to the range of Fermi energies $-3 \leqslant E_F \leqslant -1$. For other situations we have to use equation (4.3) which is computationally so demanding that a systematic study of $J(\ell)$ becomes very difficult. The numerical approach can be immediately extended to a multi-orbital band structure but the computational effort becomes prohibitive. It is therefore essential to obtain, as an alternative, asymptotic expansions for the exchange coupling of the type discussed in section 3. For this purpose we go back to equation (4.2).

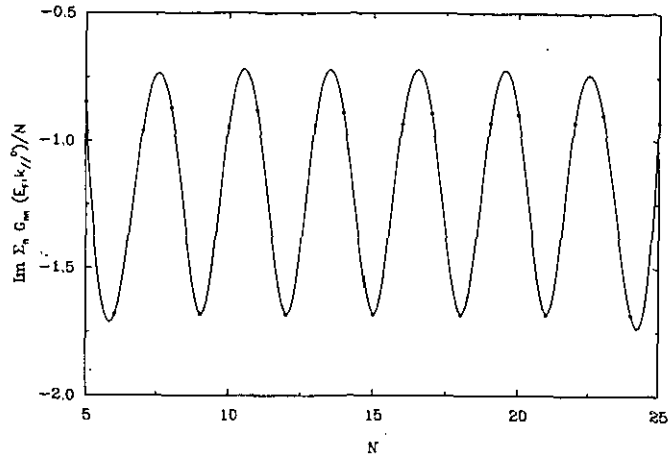

Figure 6. Imaginary part of the total normalized Green function as a function of spacer thickness N for a simple cubic tight-binding band with (100) orientation of the layers. It is evaluated at the Fermi energy $E_F = 0.5$, measured from the bottom of the spacer band, and at the extremal point $k_x = k_y = 0$ for partially confined carriers ($E_F/V = 1.25$). The solid line is a cubic spline fit to the numerical data.

In our derivation of an asymptotic formula for $J(\ell)$ we are guided by the results of [11] for the complete confinement model and by the formalism developed in section 3 for a hole-gas. The asymptotic expansion relies on the observation that, in the complete confinement model, the density of states at E_F oscillates as a function of spacer thickness and oscillations occur whenever a size-quantized level passes through the Fermi level. At the crossover from complete to partial confinement ($E = V$), the bound states evolve continuously into resonances. It follows that the density of states for E above the well also oscillates whenever a resonance crosses the Fermi level. In fact, we showed explicitly for the hole-gas model that the imaginary part of the one-electron Green function at the edge of the well ($z = \ell$) is a periodic function of ℓ. This allowed us to expand it in a Fourier cosine series. A similar expansion can be used for the tight-binding model. However, since the imaginary part of the total Green function is proportional to the spacer thickness $\ell = Na$, it is not a periodic function of N. From our discussion of the hole-gas model following equation (3.3), the relevant quantity which is expected to display a periodic behaviour is $\mathrm{Im}\sum_n G_{nn}(E, E_\parallel, N)/N$. This is illustrated in figure 6 for a simple cubic band and (100) orientation of the layers. We, therefore, represent $\mathrm{Im}\sum_n G_{nn}(E, E_\parallel, N)/N$ by a Fourier cosine series. We keep again only the oscillatory terms since the non-oscillatory part leads to the reference thermodynamic potential which has to be subtracted from Ω_{tot} in order to obtain $J(\ell)$. The oscillatory component is given by

$$(1/N)\,\mathrm{Im}\sum_n G_{nn}(E, k_\parallel, N) = \mathrm{Re}\sum_{s=1}^{\infty} a_s(E, k_\parallel)\exp[2isNa\beta(E, k_\parallel)] \tag{4.5}$$

where $\pi/\beta(E, k_\parallel)$ is the oscillation period. Transforming the summation over $k_\parallel$ into an integral over the two-dimensional Brillouin zone, we obtain

$$\Omega = \frac{k_B T N A}{4\pi^3} \sum_s \mathrm{Re} \int_{-\infty}^{\infty} \mathrm{d}E \int_{\mathrm{BZ}} \mathrm{d}k_\parallel a_s(E, k_\parallel) \times \ln[1 + \mathrm{e}^{(\mu - E)/k_B T}] \exp[2\mathrm{i}sNa\beta(E, k_\parallel)]. \tag{4.6}$$

As in section 3, the integration over $k_\parallel$ is performed using the method of stationary phase. It is clear that, for large N, the exponential factor is a rapidly oscillating function and only those regions in which $\beta(E, k_\parallel)$ is stationary with respect to $k_\parallel$ will make significant contributions to the integral. We approximate the Fourier coefficient $a_s(E, k_\parallel)$ by its value at the stationary point $k_\parallel^0$ and expand β in a Taylor series about $k_\parallel^0$ up to second-order terms to obtain

$$\Omega = \frac{k_B T A}{4\pi^2 a} \sum_s \mathrm{Re} \frac{\sigma}{s} \int_{-\infty}^{\infty} \left| \frac{\partial^2 \beta}{\partial k_x^2} \frac{\partial^2 \beta}{\partial k_y^2} \right|^{-1/2} \times a_s(E, k_\parallel^0) \ln[1 + \mathrm{e}^{(\mu - E)/k_B T}] \mathrm{e}^{2\mathrm{i}sNa\beta(E, k_\parallel^0)} \mathrm{d}E \tag{4.7}$$

where the factor σ is defined as in section 3. To perform the remaining energy integral, we first integrate by parts and then note that the region in which the Fermi function is essentially constant does not contribute to the integral because of the rapid oscillations of $\exp[2\mathrm{i}sNa\beta(E, k_\parallel^0)]$. The only contribution comes, therefore, from a narrow interval around the Fermi surface where the Fermi function varies rapidly. The evaluation of the energy integral is then straightforward and leads to the following asymptotic formula for the exchange coupling

$$J(N) = -\frac{k_B T}{8\pi N a^2} \sum_s \mathrm{Re} \frac{\sigma}{s^2} \frac{a_s(\mu, k_\parallel^0)}{\sinh[2Nas\pi(\partial\beta/\partial E)k_B T]} \times \left| \frac{\partial^2 \beta}{\partial k_x^2} \frac{\partial^2 \beta}{\partial k_y^2} \right|^{-1/2} \frac{\partial E}{\partial \beta} \mathrm{e}^{2\mathrm{i}sNa\beta(\mu, k_\parallel^0)}. \tag{4.8}$$

Before equation (4.8) can be discussed, the precise meaning of $\beta(\mu, k_\parallel^0)$ needs to be clarified. In principle, the oscillation period π/β and its derivatives could be determined numerically from the computed normalized Green function $(1/N)\,\mathrm{Im}\sum_n G_{nn}(\mu, k_\parallel^0, N)$ but the usefulness of the asymptotic formula (4.8) depends on our ability to locate stationary points of $\beta(\mu, k_\parallel^0)$. For a general (multi-orbital) band structure this is difficult. However, we propose below a working hypothesis to determine analytically the stationary points $k_\parallel^0$ and the period for any single-orbital tight-binding band and for any orientation of the sandwich provided it is parallel to a plane of reflection symmetry. Under these conditions, we showed in [11] that size-quantized energy levels for completely confined carriers are $E(k_\parallel, k_\perp = n\pi/N + 1)$, where $E(k_\parallel, k_\perp)$ is the bulk tight-binding energy and $n = 1, 2, \ldots, N$. Stationary points $k_\parallel^0$ are then simply the extremal points of the perpendicular wave vector $k_\perp(\mu, k_\parallel)$. Our working hypothesis is that, by analogy with the hole-gas model, the oscillation period for partially confined carriers is the same as for carriers confined in an infinitely deep well, i.e.

$$\beta(\mu, k_\parallel^0) = k_\perp(\mu, k_\parallel^0) \tag{4.9}$$

This appears to be justified by comparison with the numerical calculation described below.

It can be now seen that equation (4.8) complements the asymptotic expansion for J(N) derived in [11] for the complete confinement model. The oscillation period and temperature dependence of J(N) are unaffected by deconfinement since they are determined entirely by the spacer Fermi surface. On the other hand, the amplitude is controlled not only by the curvature of the spacer Fermi surface, as is the case in the complete confinement model, but it also depends critically on the exchange splitting in the magnetic layers via the Fourier component $a_s(\mu, k_\parallel^0)$ (to avoid confusion, we recall that $a_s(\mu, k_\parallel^0)$ is not the same quantity as for the hole gas since, in section 3, we Fourier analysed the Green function at the edge of the well $z = \ell$).

Given that $(1/N)\,\mathrm{Im}\sum_n G_{nn}(\mu, k_\parallel^0, N)$ is only known numerically and is defined only for discrete N, it is not as simple to determine its Fourier components $a_s(\mu, k_\parallel^0)$ as in the gas model. This is particularly true for short-period oscillations where fitting a Fourier series is not entirely unique. The most stringent test of the asymptotic expansion (4.8) is, therefore, to compare it at $T = 0\,\mathrm{K}$ with our numerical calculations for the simple cubic tight-binding model using $E_F = 0.5$ (measured from the bottom of the spacer band and given in units of $W/6$) which leads to a two-monolayer period (see figure 5). The corresponding bulk Fermi surface

$$E_F = -[\cos(k_x a) + \cos(k_y a) + \cos(k_z a)] \tag{4.10}$$

has only one extremum (minimum) at $k_x = k_y = 0$ (we take the layers to be parallel to the x–y plane). The curvature of the Fermi surface and $(\partial\beta/\partial E)$ are, therefore, easily determined from equation (4.10). Assuming partial confinement $E_F/V = 1.25$, we obtain the Fourier component $a_1(E_F, 0)$ simply by fitting a cosine wave to the computed $(1/N)\,\mathrm{Im}\sum_n G_{nn}(\mu, k_\parallel^0, N)$ shown in figure 6, thus neglecting higher harmonics. The corresponding exchange coupling $J(N)$ calculated from equation (4.8) is shown in figure 7 together with the exact numerical result obtained from equation (4.4). The agreement is remarkably good and appears to justify the assumptions leading to the asymptotic formula (4.8).

5. Conclusions

We have generalized our earlier theory [11, 12, 14] of the oscillatory exchange coupling between two transition-metal ferromagnets separated by a non-magnetic transition metal spacer to the case of a sandwich with magnetic layers which have holes both in the majority- and minority-spin bands (weak ferromagnets).

In sections 3 and 4 we investigated comprehensively the interlayer exchange coupling using hole-gas and tight-binding models for the d bands of the metals forming the sandwich. We determined the coupling numerically from the total energy difference between the ferromagnetic and antiferromagnetic configurations of the sandwich and developed general asymptotic expansions valid for large thickness ℓ of the spacer layer. The main results obtained from our numerical studies and from the asymptotic expansions are essentially the same for both models.

(i) The oscillation period and temperature dependence of the interlayer coupling are determined entirely by the properties of the spacer layer Fermi surface and

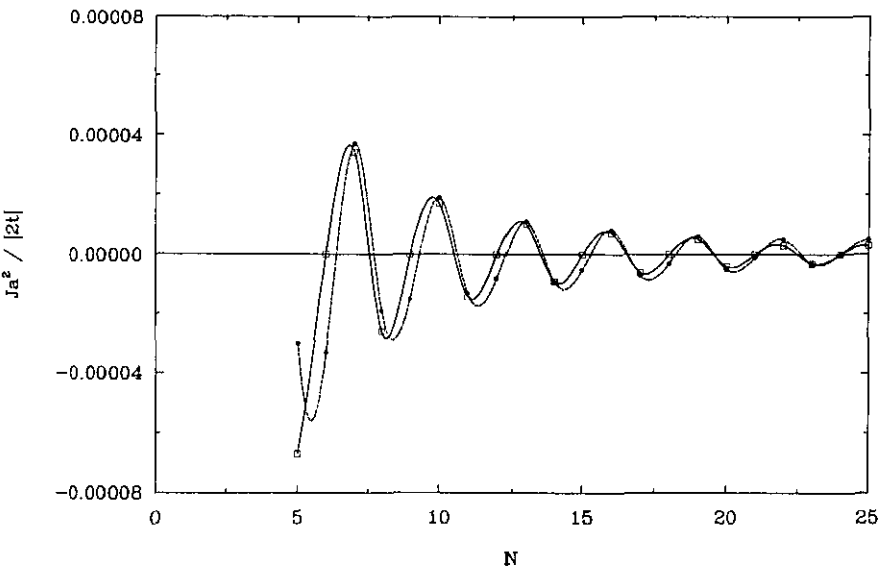

Figure 7. Comparison between the asymptotic behaviour (solid curve) of the exchange coupling $J(N)$ obtained from equation (4.8) for a simple cubic tight-binding band and the exact result (dashed curve) obtained calculating the thermodynamic potential numerically. The parameters are chosen so as to correspond to partial confinement of the magnetic carriers ($E_F/V = 1.25$). In the asymptotic expansion (4.8) the Fourier coefficient $a_1(E_F, 0) = 0.15$ is simply obtained from the amplitude of the oscillations in $\mathrm{Im} \sum_n G_{nn}(E_F, k_\parallel^0, N)/N$ shown in figure 6.

are thus independent of the exchange splitting (magnetization) in the ferromagnetic layers. (As in [11, 12], we refer here to the Fermi surface of d electrons; sp electrons are not included in our model).

(ii) The overall amplitude of the exchange coupling is determined by two factors: the curvature of the Fermi surface in the non-magnetic spacer layer and the bulk exchange splitting in the ferromagnetic layers. When we move, keeping a fixed Fermi energy, from a ferromagnet with an infinitely large exchange splitting (the only case considered in [11, 12]) to a 'just strong' ferromagnet, the amplitude remains constant but it drops dramatically as soon as the ferromagnet becomes weak (holes in the majority-spin band).

(iii) The asymptotic formula for the hole-gas model valid to order $1/\ell^2$ shows that the phase of oscillations in the exchange coupling changes through 2π as we move from an infinitely strong ferromagnet to a 'just strong' ferromagnet but then locks at zero at the crossover to a weak ferromagnet and remains independent of the exchange splitting. This latter result is also obtained in our numerical calculations for a single-orbital tight-binding band.

(iv) Numerical studies both for the gas and tight-binding models show, however, that there is a definite phase shift between the oscillations in the exchange coupling obtained for very strong and weak ferromagnets. The same result is obtained when the asymptotic expansion for the hole-gas model is extended to include the terms in $1/\ell^3$. However, the phase shifts obtained for the hole-gas and tight-binding models are different indicating that the phase is a model-dependent quantity.

We pointed out in the introduction that our most recent numerical calculations of the exchange coupling for Fe/Cr/Fe sandwich employing a canonical five-orbital d band and assuming an infinitely large exchange splitting grossly overestimate the oscillation amplitude and have a wrong phase. The results of sections 3 and 4 strongly suggest that both these discrepancies may be removed when the assumption of the infinitely large exchange splitting is relaxed. This requires generalization of the present theory to a multi-orbital band structure. Although such a generalization is possible both for the numerical approach and the asymptotic expansions, the computational effort involved in the former is prohibitive. Asymptotic expansions appear, therefore, much more promising.

Finally we wish to discuss a connection between our theory and RKKY. Our conclusion that the oscillation periods are characteristic of the spacer metal, whereas the amplitude and phase depend strongly on the matching between the bands in the spacer and ferromagnet, is similar to that of Bruno [18]. He calculates the coupling between two magnetic transition-metal monolayers immersed in a simple or noble metal. A synthesis of our work and Bruno's, applicable to both transition- and noble-metal spacers, will be achieved when our tight-binding calculations are further extended to include hybridization of the d band with the sp bands.

Acknowledgments

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Appendix

In this appendix we give an alternative simpler method of calculating the exchange coupling between the ferromagnetic layers of a sandwich using a hole-gas model. In contrast to the formalism of section 3, the method presented here allows us to go one step further and include terms in $1/\ell^3$ in the asymptotic expansion of $J(\ell)$. However, it has the serious drawback that it is not generalizable to an arbitrary band; also it is only applicable to the exchange coupling at zero temperature.

The Hamiltonian for a hole-gas in the presence of a potential well of width ℓ in the z direction and depth V can be written as

$$H = -(\hbar^2/2m)\nabla^2 + V - V\Theta(z) + V\Theta(z-\ell) \tag{A1}$$

where $\Theta(z)$ is the step function having unit value when $z \geqslant 0$ and zero otherwise. The basis functions $|k_\parallel, z'\rangle$ we use are written in a mixed momentum-position representation, with normalization

$$\langle k'_\parallel, z''|k_\parallel, z'\rangle = \delta_{k_\parallel, k'_\parallel}\delta(z''-z'). \tag{A2}$$

As in section 2, we first calculate $\mathrm{d}\Omega_{\mathrm{tot}}/\mathrm{d}\ell$. At zero temperature it reads

$$\frac{\mathrm{d}\Omega_{\mathrm{tot}}}{\mathrm{d}\ell} = \int_0^{E_F} (E - E_F)\frac{\mathrm{d}\mathcal{D}(\ell, E)}{\mathrm{d}\ell}\,\mathrm{d}E \tag{A3}$$

where the zero of energy has been chosen to be at the bottom of the well. The density of states $\mathcal{D}(\ell, E)$ is given by

$$\mathcal{D}(\ell, E) = (-1/\pi)\,\mathrm{Im}\,\mathrm{Tr}(E - H + \mathrm{i}\eta)^{-1} \tag{A4}$$

where η is an infinitesimal positive quantity and the trace consists of a summation over $\boldsymbol{k}_\parallel$ and an integration over z. Since $(E - H + \mathrm{i}\eta)^{-1}$ depends on ℓ only through the Hamiltonian H, it is easy to show that

$$\frac{\mathrm{d}\mathcal{D}(E,\ell)}{\mathrm{d}\ell} = -\frac{1}{\pi}\,\mathrm{Im}\sum_{\boldsymbol{k}_\parallel}\int \mathrm{d}z\langle \boldsymbol{k}_\parallel, z|(E - H + \mathrm{i}\eta)^{-1}\frac{\partial H}{\partial \ell}(E - H + \mathrm{i}\eta)^{-1}|\boldsymbol{k}_\parallel, z\rangle. \tag{A5}$$

It follows from equation (A1) that

$$\frac{\partial H}{\partial \ell} = -V\delta(z - \ell) = -V|\ell\rangle\langle\ell| \tag{A6}$$

which yields

$$\frac{\mathrm{d}\mathcal{D}(E,\ell)}{\mathrm{d}\ell} = \frac{V}{\pi}\,\mathrm{Im}\sum_{\boldsymbol{k}_\parallel}\langle \boldsymbol{k}_\parallel, \ell|(E - H + \mathrm{i}\eta)^{-2}|\boldsymbol{k}_\parallel, \ell\rangle \tag{A7}$$

where we have used the closure relation $\int dz|z\rangle\langle z| = 1$ to perform the integration over z. Equation (3.1) follows immediately from equation (A7).

To perform the integration over $\boldsymbol{k}_\parallel$, we do not use here the method of stationary phase but turn the summation into an integral involving the two-dimensional density of states $\mathcal{D}_{2D}(E_\parallel)$. Recognizing that for a parabolic band $\mathcal{D}_{2D}(E_\parallel) = (1/2\pi)(m/\hbar^2)$ is a constant, we can write $\mathrm{d}\Omega_{\mathrm{tot}}/\mathrm{d}\ell$ in the form

$$\begin{aligned}\frac{\mathrm{d}\Omega_{\mathrm{tot}}}{\mathrm{d}\ell} &= -\frac{V}{\pi}\mathcal{D}_{2D}(E_\parallel)\int_0^\infty \mathrm{d}E_\parallel \int_0^{E_F}(E - E_F)\\ &\quad\times\frac{\partial}{\partial E}\,\mathrm{Im}\langle\ell|(E - E_\parallel - H(\ell) + \mathrm{i}\eta)^{-1}|\ell\rangle\,\mathrm{d}E\\ &= \frac{V}{\pi}\mathcal{D}_{2D}(E_\parallel)\int_0^\infty \mathrm{d}E_\parallel \int_0^{E_F}(E - E_F)\\ &\quad\times\frac{\partial}{\partial E_\parallel}\,\mathrm{Im}\langle\ell|(E - E_\parallel - H(\ell) + \mathrm{i}\eta)^{-1}|\ell\rangle\,\mathrm{d}E\end{aligned} \tag{A8}$$

where $H(\ell)$ is the Hamiltonian in the direction perpendicular to the sandwich and, in the last equation, we used the symmetry between E and $E_\parallel$ to transform the derivative with respect to E into a derivative with respect to $E_\parallel$. Integrating over $E_\parallel$ and introducing the one-electron Green function at the edge of the well, $G(\ell, \ell, E, E_\parallel = 0) = \langle\ell|(E - H + \mathrm{i}\eta)^{-1}|\ell\rangle$, we finally get

$$\frac{\mathrm{d}\Omega_{\mathrm{tot}}}{\mathrm{d}\ell} = -\frac{V}{\pi}\mathcal{D}_{2D}(E_\parallel)\int_0^{E_F}(E - E_F)\,\mathrm{Im}\,G(\ell, \ell, E)\,\mathrm{d}E. \tag{A9}$$

The one-electron Green function at the edge of the well can easily be calculated analytically. Above the well ($E > V$), it is given by equation (3.3) with $E_\parallel = 0$.

Inside the well ($E < V$), the imaginary part of the Green function reduces to a sum of delta functions corresponding to size-quantized energy levels. It is given by

$$\operatorname{Im} G(\ell, \ell, E) = -\frac{\pi}{V}\beta \sum_n \delta(\beta\ell + \psi - n\pi) \tag{A10}$$

where $\beta = (2mE/\hbar^2)^{1/2}$ and the phase shift ψ is a function of energy defined in equation (3.11). $\operatorname{Im} G(\ell, \ell, E)$ is, of course, a periodic function of ℓ and can be expanded in a Fourier series. This leads directly to

$$\frac{\mathrm{d}\Omega}{\mathrm{d}\ell} = \frac{\mathcal{D}_{2D}(E_\parallel)}{\pi}\left(\frac{\hbar^2}{m}\right)^2 \sum_{p=1}^{\infty} \int_0^{k_F} (\beta^2 - k_F^2)\beta^2 \cos[2p(\beta\ell + \psi)]\,\mathrm{d}\beta. \tag{A11}$$

Here we write Ω rather than Ω_{tot} since we have dropped the non-oscillatory reference component. Successive integrations by parts of equation (A11) followed by integration with respect to ℓ then yield the exchange coupling $J(\ell)$ to any power in $1/\ell$. To order $1/\ell^2$, we obtain equation (3.10) but it is now possible to include higher-order terms. A similar procedure can be followed to obtain the exchange coupling at $T = 0$K when the Fermi level lies above the top of the well. As mentioned in section 2, when only terms in $1/\ell^2$ are included in the asymptotic expression for $\mathrm{d}\Omega/\mathrm{d}\ell$, there appears a phase shift between the asymptotic results and the numerical results obtained from equation (3.2). To investigate this discrepancy we have calculated terms in $1/\ell^3$ in the expression for $\mathrm{d}\Omega/\mathrm{d}\ell$. We do not display this result here since it is easily obtained but leads to rather lengthy expressions. When the higher-order terms are included the apparent phase shift disappears.

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