Exponential behavior of the interlayer exchange coupling across nonmagnetic metallic superlattices

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It is shown that the coupling between magnetic layers separated by nonmagnetic metallic superlattices can decay exponentially as a function of the spacer thickness N, as opposed to the usual N^{-2} decay. This effect is due to the lack of constructive contributions to the coupling from extended states across the spacer. The exponential behavior is obtained by properly choosing the distinct metals and the superlattice unit cell composition. [S0163-1829(98)01337-X]

The alignment of the magnetizations of metallic layers separated by nonmagnetic metallic spacers oscillates between parallel and antiparallel as the distance N between the magnetic layers is varied. This oscillatory interlayer exchange coupling $J(N)$ has been intensively investigated both experimentally and theoretically.[1,2] At zero temperature and for sufficiently thick metallic spacers, the amplitude of J decays usually as $1/N^2$, and its oscillation periods depend on the geometry of the spacer Fermi surface (FS).[3–7] Such a behavior has been regarded as characteristic of crystalline metallic spacers. In fact, simple theoretical arguments show that the coupling across insulating materials decays exponentially with N,[8,10] the reason being the absence of extended electronic states within the insulating spacer with energy equal to the chemical potential.

There are general rules which provide a systematic way for determining the oscillation periods of J across metallic spacers.[4–6] In their simplest form they correspond to the RKKY criterion, which states that the periods are given by critical spanning wave vectors along the growth direction linking two points of the bulk spacer FS with antiparallel velocities.[4] Recently, it has been suggested that the periods of J across nonmagnetic metallic superlattices can be altered in a controllable way by changing the superlattice composition, and, hence, its FS.[11] In this paper we show that it is possible to find an exponentially decaying $J(N)$ across nonmagnetic metallic superlattices. Such a behavior can be obtained by properly choosing the superlattice constituent materials and unit cell composition in such a way that the superlattice FS shows no critical wave vectors in the direction perpendicular to the layers. In this case, despite the metallic character of the spacer, the contributions to the coupling coming from extended states interfere destructively.

The systems we examine are composed of two semi-infinite ferromagnetic metals separated by a nonmagnetic metallic superlattice. The superlattice unit cell consists of two layers, made of metals A and B, containing N_A and N_B atomic planes, respectively. We have calculated J as a function of the number of atomic planes in the spacer. However, as far as the periods are concerned, it is only when probed at regular intervals of the supercell size ($N_s = N_A + N_B$ atomic planes) that the coupling reflects the structure of the spacer superlattice FS.[11] Therefore, to highlight the oscillation periods which are associated with the superlattice FS, when we show our calculated results for $J(N)$ we indicate one subset of N values that are equally spaced by the supercell size N_s.

Having in mind simple and noble metals, which for most purposes can be regarded as one-band materials, we consider that the multilayer electronic structure is described by the single-band tight-binding model on a simple cubic lattice with nearest-neighbor hoppings only. We assume that the hopping t is the same throughout the multilayer system, and choose the unit of energy so that $t = 1/2$. We consider the atomic planes oriented in the (001) direction, and set the on-site energies in the magnetic layers equal to $\epsilon_M^{\uparrow} = -0.15$ and $\epsilon_M^{\downarrow} = 0.15$, for $\uparrow$ and $\downarrow$ spin electrons, respectively. Our calculations of the interlayer exchange coupling J, defined as the difference in total energy per surface atom between the antiferromagnetic and ferromagnetic configurations of the system, have been performed at zero temperature, and are based on the formalism developed in Refs. 7 and 12.

We first look at one spacer superlattice case where the usual $1/N^2$ behavior of $J(N)$ occurs. We consider $N_A = N_B = 1$, and take the on-site energies of metals A and B to be $\epsilon_A = -0.4$ and $\epsilon_B = 0.2$, respectively. The calculated results for $J(N)$ are presented in Fig. 1(a). The open circles indicate one of the subsets of points corresponding to values of N separated by $N_s = 2$. We can see that they oscillate with a single period (depicted by the dashed line) of $\approx 6N_s$ atomic planes. The other subset of points has the same oscillation period, except for a phase shift. The short-period oscillation followed by the solid line does not reflect any fundamental period related to the spacer FS. This line simply connects results for spacer thicknesses differing by one atomic plane, joining points of different subsets which have a common oscillation period but distinct phases. It is clear from Fig. 1(b), where $J \times N^2$ is plotted against N, that the amplitude of J decays as $1/N^2$. The period followed by the open circles in Fig. 1(a) agrees perfectly with what we obtain from the critical wave vectors of the superlattice FS displayed in Fig. 1(c), as expected.

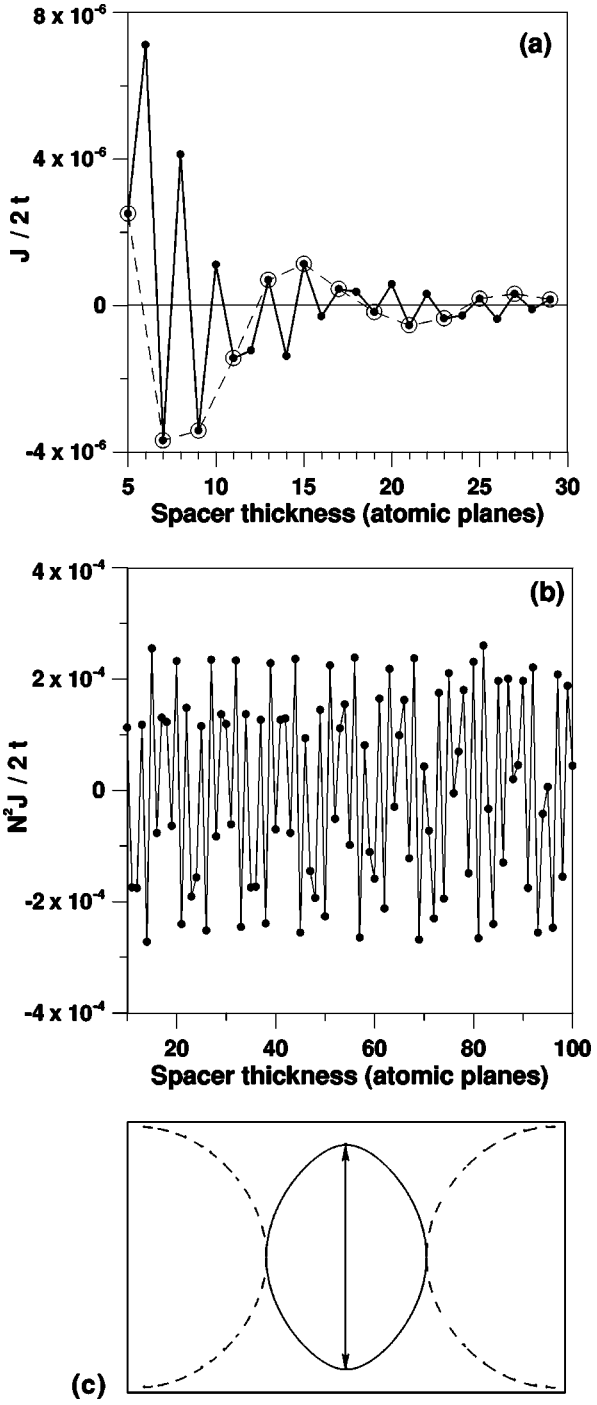

FIG. 1. (a) Calculated coupling J as a function of spacer thickness N. Solid and open circles mark the superlattice atomic planes and unit cells, respectively. (b) N^2J as a function of N. (c) Superlattice FS. The rectangle is a (100) cross section of the superlattice first Brillouin zone. Solid lines represent the real FS and dashed line the CFS. All results are for $N_A=N_B=1$, $\epsilon_A^0=-0.4$, and $\epsilon_B^0=0.2$.

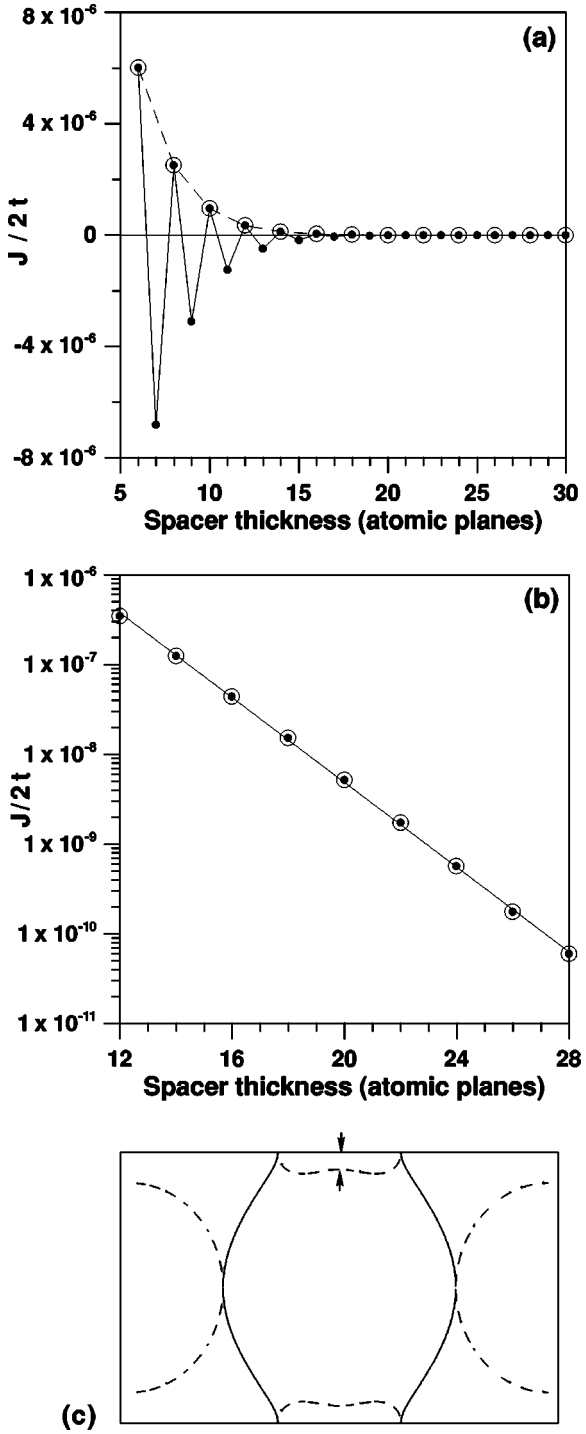

FIG. 2. (a) Calculated coupling J as a function of spacer thickness N. Solid and open circles mark the superlattice atomic planes and unit cells, respectively. (b) $|J|$ as a function of N; only the open circles are shown. (c) Superlattice FS. The rectangle is a (100) cross section of the superlattice first Brillouin zone. Solid lines represent the real FS and dashed line the CFS. All results are for $\epsilon_A^0-0.4$ and $\epsilon_B^0=-0.9$.

We now show that a completely different behavior of $J(N)$ can be obtained, by simply replacing metal B in the superlattice by another metal. It is well known that different choices of spacer materials can lead to different oscillation periods, amplitudes, and phases of the oscillatory interlayer coupling, but provided the metallic character of the spacer is preserved, the coupling amplitude is expected to decay always according to a power law for sufficiently large values of N. For metallic spacer superlattices, however, this is not generally true, and we will prove that an exponentially decaying $J(N)$ can be found in some cases. We consider, as an example, the same superlattice unit cell composition as before, i.e., $N_A=N_B=1$, but replace metal B by another in which $\epsilon_B^0=-0.9$. The calculated results of $J(N)$ for this case

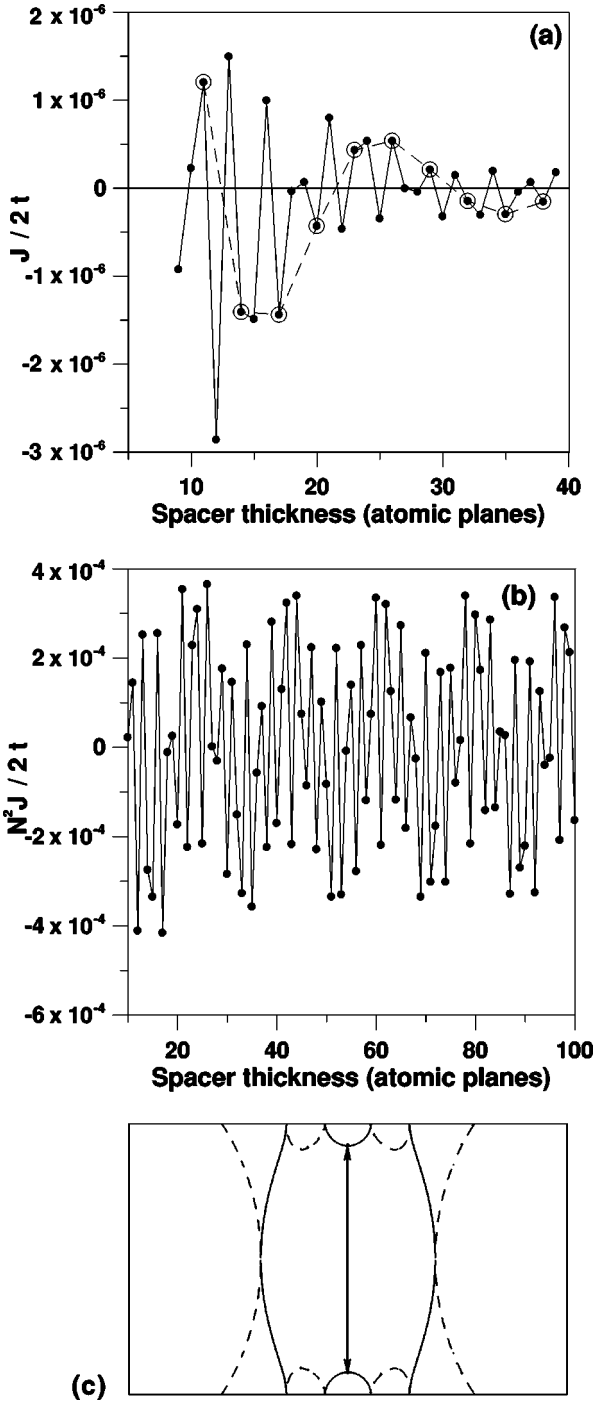

FIG. 3. (a) Calculated coupling J as a function of spacer thickness N. Solid and open circles mark the superlattice atomic planes and unit cells, respectively. (b) N^2J as a function of N. (c) Superlattice FS. The rectangle is a (100) cross section of the superlattice first Brillouin zone. Solid lines represent the real FS and dashed line the CFS. All results are for $N_A=2, N_B=1$, $\epsilon_A^0=-0.4$, and $\epsilon_B^0=0.2$.

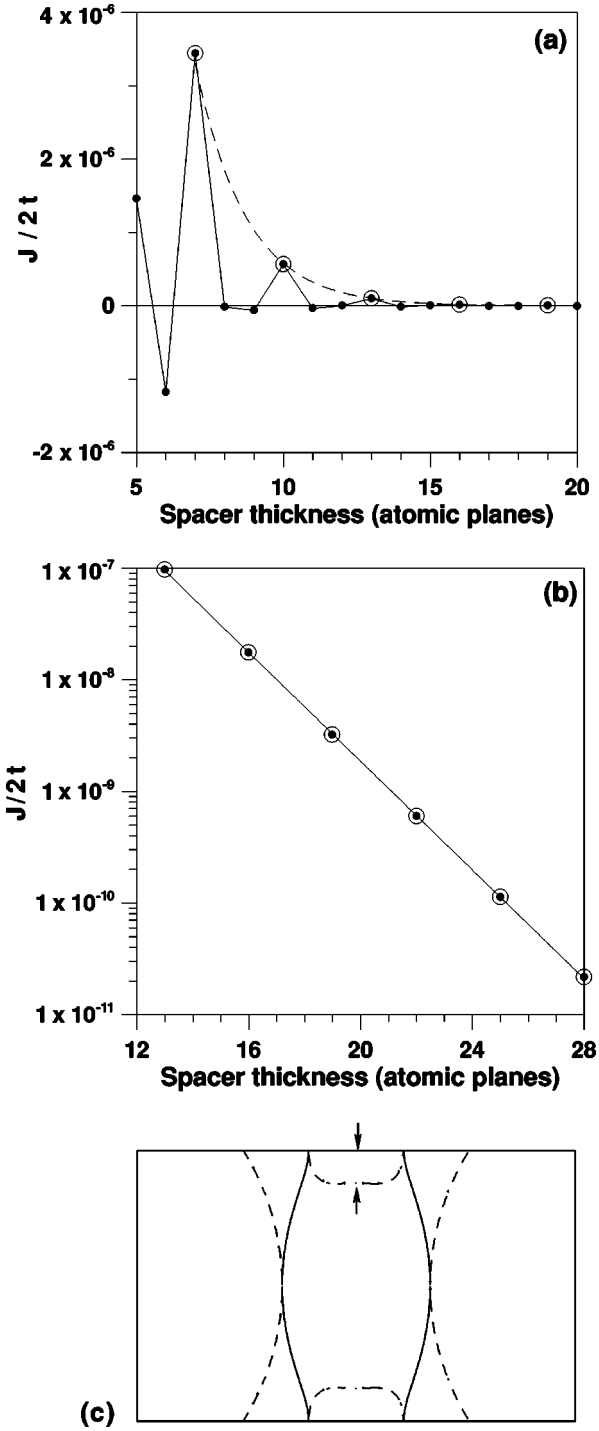

FIG. 4. (a) Calculated bilinear coupling J as a function of spacer thickness N. Solid and open circles mark the superlattice atomic planes and unit cells, respectively. (b) $|J|$ as a function of N; only the open circles are shown. (c) Superlattice FS. The rectangle is a (100) cross section of the superlattice first Brillouin zone. Solid lines represent the real FS and dashed line the CFS. All results are for $N_A=2, N_B=1$, $\epsilon_A^0=0.2$, and $\epsilon_B^0=-0.4$.

are presented in Fig. 2(a). As before, open circles indicate one subset of equally spaced values of N differing by N_s. These points clearly show a much faster decreasing coupling as a function of the spacer thickness. In fact, their plot in logarithmic scale, as in Fig. 2(b), makes it evident that J decays exponentially in this case. The other subset of points, corresponding to odd numbers of atomic planes, exhibits the same exponential rate of decay. Such an exponential behavior can be understood by analyzing the corresponding spacer superlattice FS, which is represented by the solid line in Fig. 2(c). First we notice that, in contrast with the previous case, this superlattice FS shows no critical spanning vectors satisfying the criteria for obtaining an oscillatory coupling.

Therefore, the extended states of the spacer superlattice do not interfere constructively giving no sizeable contributions to the coupling asymptotically. It is worth mentioning that both the chosen metals A and B, separately, have bulk Fermi surfaces which satisfy those criteria. Hence, across either of these pure metals, the coupling would be oscillatory and its amplitude would follow the usual $1/N^2$ asymptotic behavior. However, our particular choice has produced a superlattice FS which shows no critical wave vectors, thereby leading to an exponentially decreasing coupling. This results from the fact that the interlayer exchange coupling is basically regulated by a few critical wave vectors of the spacer FS and is sensitive to variations of the spacer FS around these states.

The exponential rate of decay of the coupling can be obtained from the so-called complex Fermi surface (CFS),[9] which is associated with evanescent states in the spacer having complex wave vectors. The CFS's are shown by the dashed lines in Figs. 1(c) and 2(c). In order to preserve continuity between the real and complex FS sheets, we have added the real part of the wave vector k_z to the complex part of the FS when drawing the latter.[10] A simple extension of the stationary phase method states that when the real FS shows no critical wave vectors, the dominant contributions to the coupling come from the critical points of the complex FS. In this case, all contributions from the real part of the FS interfere destructively in the asymptotic region. Thus, we are left with only the exponentially decaying contributions coming from the complex part of the FS, the most important being the stationary one with the smallest rate of decay, which is indicated by arrows in Fig. 2(c). One can easily verify that the magnitude of the imaginary part of the critical wave vectors corresponds to the slope of the line in Fig. 2(b). In other words, rather than determining the periods with which the coupling oscillates, critical wave vectors of the complex part of the FS indicate how fast the exponential decay is.

Having shown that it is possible to find an exponentially decaying coupling by properly choosing the metals of which the spacer superlattices are made, we now show that the same effect can be obtained by fixing a pair of metals and varying the superlattice unit cell composition. To illustrate this, we take the same metals as in the first case, i.e., those corresponding to $\epsilon_A = -0.4$ and $\epsilon_B = 0.2$, but consider larger supercells. First we look at a superlattice with $N_A = 2$ and $N_B = 1$ (AAB type of cell), and later we consider another in which $N_A = 1$ and $N_B = 2$ (ABB type of cell). The calculated results of $J(N)$ for the first case are presented in Fig. 3(a), where we have singled out one subset of N values differing by integer multiples of $N_s = 3$. It is evident that in this case the coupling exhibits the usual behavior, with the amplitude decaying asymptotically as $1/N^2$, as confirmed by Fig. 3(b). The corresponding superlattice FS, shown in Fig. 3(c), clearly has a critical wave vector which regulates the asymptotic oscillatory behavior of the coupling. However, when we look in Fig. 4(a) at the coupling across the spacer superlattice which has the ABB type of structure, we imediately notice that it decreases much faster than in the previous case. The logarithmic plot presented in Fig. 4(b) confirms that the coupling amplitude decays exponentially in this case. Such exponential behavior agrees with the fact that the corresponding superlattice FS, shown in Fig. 4(c), has no critical wave vectors but in the CFS sheet, and the extremum that regulates the coupling rate of decay is also indicated by arrows in this figure.

In conclusion, we have shown that exponentially decaying interlayer couplings as a function of the spacer thickness can be obtained across metallic superlattices. They result from the absence of real critical wave vectors associated with the superlattice FS. In this case the existing extended states interfere destructively reducing the coupling rapidly as the superlattice thickness increases. The effect is due to quantum interferences generated by the superlattice interfaces, and can be obtained either by a proper selection of the metals involved or by adjusting the superlattice composition. The states which effectively contribute to the coupling in this case are evanescent and are selected from critical wave vectors of the complex part of the FS. Spacer superlattices made of monovalent metals, whose Fermi surfaces are relatively simple, are good candidates for presenting such a behavior. This remarkable change of response to the superlattice composition is a special feature of the interlayer coupling which is a quantity that depends basically on just a few critical wave vectors. Other properties, such as the strength of the giant magnetoresistence effect, for instance, are not expected to be so sensitive to local changes of the spacer FS because they depend on it as a whole, not just on specific portions like the interlayer coupling.

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