Tunneling theory for exchange coupling between two ferromagnets separated by an amorphous-semiconducting barrier

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We have developed a tunneling theory for the exchange coupling between two ferromagnets separated by an amorphous-insulating barrier. It includes direct non-spin-flip tunneling, assisted non-spin-flip tunneling, and assisted spin-flip tunneling, which favor the ferromagnetic coupling in the long range of the barrier thickness, middle-range antiferromagnetic coupling, and short-range ferromagnetic coupling. The exchange coupling oscillates from a ferromagnetic type to an antiferromagnetic one and back to a ferromagnetic one with the increasing of the barrier thickness if the spin-flip tunneling is strong enough; otherwise, it is always ferromagnetic. The results are qualitatively in agreement with the experimental observations on Fe/Si/Fe and Fe/Ge/Fe trilayers. [S0163-1829(96)03426-1]

The discovery of an oscillatory exchange interaction between ferromagnets through a nonmagnetic metallic spacer has recently excited the investigation on the exchange coupling between ferromagnets through an amorphous-semiconducting spacer. This has indeed been verified first by Toscano *et al.*[1] in a sandwich structure of Fe/Si/Fe, and latterly by Füllerton *et al.*[2,3] and Foiles *et al.*[4] in Fe/Si superlattices. The exchange coupling is always of ferromagnetic type for Fe/SiO/Fe (Ref. 5) and Fe/Ge/Fe (Ref. 6) trilayers, changes from ferromagnetic type to antiferromagnetic one for Fe/Si superlattices,[2–4] and oscillates from ferromagnetic (FM) type to antiferromagnetic (AF) type and back to ferromagnetic (FM) type for Fe/Si/Fe (Refs. 1, 6, and 7) with the increase of the thickness of the corresponding spacer. The experiment[6] also indicates *a*-Si contains a higher density of defects as compared with *a*-Ge. Additionally, the coupling is heat activated[5–7] and photon induced,[8] that is to say, it increases with increasing temperatures,[5–7] and may be induced by illumination of visible light.[8]

Two models have been proposed to explain those phenomena: One is the so-called quantum-well theory for magnetic tunneling junction due to Slonczewski,[9] the essence of which is to construct, from solutions of Schrödinger's equation, stationary wave functions within each of the three regions of the tunneling junction (barrier, left and right electrodes) by matching them together at the two barrier-electrode boundaries such that they and their derivatives are continuous at these points, the spin-independent potentials in the three regions and internal exchange molecular fields in the two FM electrodes being treated within the mean-field approximation. It predicts AF coupling for small gaps in contradiction to the experimental observation of Ref. 6 where *a*-Ge exhibits FM coupling in spite of its smaller gap as compared to *a*-Si which exhibits AF coupling; the other model is due to Bruno.[10,11] The system under his consideration is also a sandwich of two ferromagnets separated by a paramagnetic spacer layer, after the perturbations due to the two ferromagnets are handled by using the *t*-matrix formalism, the coupling is expressed in terms of the spin asymmetry of the reflection at the paramagnetic-ferromagnetic interfaces. It succeeds in obtaining an exchange coupling which increases with increasing temperature, but, regrettably, it also predicts AF coupling for small gaps because it reduces to Slonczewski's result at zero temperature,[11] so this mechanism cannot account for the experimental phenomena as well.[6]

For the amorphous semiconductors such as *a*-Si, *a*-Ge, etc., there exist large numbers of the localized defect states, according to the viewpoint of Mott and Davis,[12] they build a narrow band in the energy gap where the Fermi level is pinned, as sketched in Fig. 1. It is well known that those localized states in the gap near the Fermi level play a very important role in various physical processes present in amorphous semiconductors, such as transport properties, light scattering, absorption, etc., thus, it is reasonable to believe[6,7,10] that the localized states in the amorphous-semiconducting barrier are able to impose a strong influence

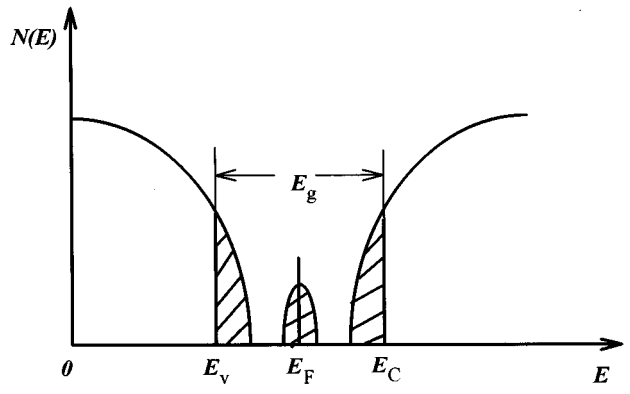

FIG. 1. Density of states $N(E)$ as a function of energy E in amorphous semiconductors. Here E_C and E_V denote the mobility edges of the down and up bands, respectively, E_g the energy gap, and E_F the Fermi level.

on the exchange interaction between the two FM electrodes. However, the quantum-well theory of Slonczewski[9] and Bruno's t-matrix formalism[10,11] are inconvenient to incorporate this influence, therefore, we turn to the transfer Hamiltonian approach[13] and postulate an assisted tunneling mechanism for the exchange coupling between ferromagnets separated by an amorphous semiconductor.

Our theory is based on the direct tunneling and the indirect tunneling arising from the Coulomb interaction between the tunneling electrons and the electrons in the localized states of the amorphous-semiconducting barrier. The direct tunneling Hamiltonian, which is the same as the usual one accountable for metal-insulator-superconductor tunneling junction, is non-spin-flip and produces FM coupling. The Coulomb interaction results in both the indirect tunneling assisted by spin-flip scattering of tunneling electrons with the magnetic moments of the electrons in the localized states which produces AF coupling between the two FM electrodes, and the indirect tunneling assisted by the transition of electron from one localized state to another localized state which is also non-spin-flip and produces FM coupling across the barrier. Apparently, our theory can account the influence of the defect states in the amorphous barrier on the exchange coupling by a natural method. It depends upon the concentration of the defect states whether the coupling across the barrier oscillates.

Initially, let us consider a tunneling system consisting of two semi-infinite metallic ferromagnets sandwiched with an amorphous semiconductor, as depicted in Fig. 2. According to the transfer Hamiltonian approach,[13] the Hamiltonian for the system takes the following form:

$$H=\sum_i \frac{\mathbf{p}_i^2}{2m}+\sum_i u(\mathbf{r}_i)+\frac{1}{2}\sum_{ij} v(\mathbf{r}_i-\mathbf{r}_j), \tag{1}$$

where $v(\mathbf{r}_i-\mathbf{r}_j)$ represents the Coulomb interaction, and $u(\mathbf{r}_i)$ the single-electron potential. Here, we would like to emphasize that the height U of the potential $u(\mathbf{r})$ in the barrier region originates in the difference of the energy gap of the semiconducting barrier and the Fermi level of the electrodes, the smaller the gap is, the lower the height U is, and the weaker the attenuations of the wave functions are in the barrier region (see Fig. 2).

In the second-quantized representation, the Hamiltonian (1) is reformulated as

$$H=\int d\mathbf{r}\psi^\dagger\left[\frac{\mathbf{p}^2}{2m}+u(\mathbf{r})\right]\psi(\mathbf{r}) + \frac{1}{2}\int\int d\mathbf{r}_1 d\mathbf{r}_2 \psi^\dagger(\mathbf{r}_1)\psi^\dagger(\mathbf{r}_2)v(\mathbf{r}_1-\mathbf{r}_2)\psi(\mathbf{r}_2)\psi(\mathbf{r}_1), \tag{2}$$

where $\psi(\mathbf{r})$ stands for electron field operator, it can be expanded in terms of states $\phi_{l\mathbf{k}}(\mathbf{r})$, $\phi_{r\mathbf{q}}(\mathbf{r})$, and $w(\mathbf{r}-\mathbf{R}_i)$, as described in Fig. 2,[13] they represent, respectively, complete sets of states on the left and right sides of the junction and overlap in the barrier region itself, and the localized defect states near the Fermi energy in the amorphous barrier. Thus,

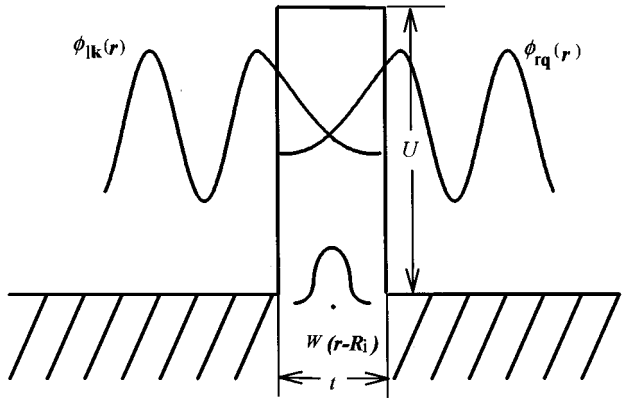

FIG. 2. Tunneling junction with two FM electrodes sandwiched by an amorphous semiconductor. Separate wave functions $\phi_{i\mathbf{k}}(\mathbf{r})$ and $\phi_{r\mathbf{q}}(\mathbf{r})$ are, respectively, wave functions in the left and right regions of the structure and decay exponentially into the barrier and beyond into the opposite electrode, $w(\mathbf{r}-\mathbf{R}_i)$ represents the localized defect states in the barrier region. U represents the height of the potential in the barrier, and t the barrier thickness.

$$\psi(\mathbf{r})=\sum_{\mathbf{k}\sigma} d_{\mathbf{k}\sigma}\phi_{l\mathbf{k}}(\mathbf{r})\eta_\sigma+\sum_{\mathbf{q}\sigma} f_{\mathbf{q}\sigma}\phi_{r\mathbf{q}}(\mathbf{r})\eta_\sigma + \sum_{i\sigma} c_{i\sigma}w(\mathbf{r}-\mathbf{R}_i)\eta_\sigma, \tag{3}$$

where η_σ denotes the spin wave function, $d_{\mathbf{k}\sigma}$ destroys an electron of wave vector $\mathbf{k}$ and spin projection σ on the left, $f_{\mathbf{q}\sigma}$ destroys an electron of wave vector $\mathbf{q}$ and spin projection σ on the right, and $c_{i\sigma}$ destroys a localized state of spin σ at site $\mathbf{R}_i$ in the barrier. Inserting Eq. (3) into Eq. (2), one finds that the Hamiltonian (2) can be grouped into the terms describing the electrodes separately and those describing the tunneling:

$$H=H_0+H_1+H_2+H_3+H_4+H_5, \tag{4}$$

the rest terms of the Hamiltonian being neglected because they have less effect on the tunneling. The first term in Eq. (4)

$$H_0=\sum_{\mathbf{k}\sigma}\epsilon_{\mathbf{k}\sigma}d^\dagger_{\mathbf{k}\sigma}d_{\mathbf{k}\sigma}+\sum_{\mathbf{q}s}\zeta_{\mathbf{q}s}f^\dagger_{\mathbf{q}s}f_{\mathbf{q}s} \tag{5}$$

represents the energies of the electrons on the left and right FM electrodes where the splittings of energy bands arising from the Coulomb interaction have been included. We caution that each of the two FM electrodes may, now, have the magnetic quantization axis of itself and differ from each other by an angle. The second term

$$H_1=\sum_{\mathbf{kq}}\sum_\sigma (T^{(1)}_{\mathbf{kq}}d^\dagger_{\mathbf{k}\sigma}f_{\mathbf{q}\sigma}+\text{H.c.}) \tag{6}$$

is the tunneling Hamiltonian usually used, it describes direct or nonassisted tunneling processes where the tunneling electrons do not interact with the localized states in the barrier when they transfer from one FM electrode to the other. The rest of the parts of Eq. (4), which come from the Coulomb interaction between the tunneling electrons and the localized

states in the barrier, describe the indirect or assisted tunneling processes where the tunneling electrons interact with the localized states in the barrier when they transfer from one FM electrode to the other. The third term

$$H_2=\sum_{\mathbf{kq}}\sum_{\sigma}\sum_{i}\left(T^{(2)}_{i\mathbf{kq}}-\frac{1}{2}T^{(3)}_{i\mathbf{kq}}\right)n_i(d^{\dagger}_{\mathbf{k}\sigma}f_{\mathbf{q}\sigma}+f^{\dagger}_{\mathbf{k}\sigma}d_{\mathbf{q}\sigma}) \quad (7)$$

stands for the interaction between the charge of the tunneling electrons and the charges of the localized states in the barrier where $n_i=\Sigma_{\sigma}c^{\dagger}_{i\sigma}c_{i\sigma}$, this charge-charge interaction should be compensated by the contribution from the positive background because the whole barrier is neutral, so we omit it in the following. The fourth term

$$\begin{aligned}H_3=-\sum_{\mathbf{kq}}\sum_{i}T^{(3)}_{i\mathbf{kq}}\{&S^{z}_{i}[(d^{\dagger}_{\mathbf{k}\uparrow}f_{\mathbf{q}\uparrow}-d^{\dagger}_{\mathbf{k}\downarrow}f_{\mathbf{q}\downarrow})\\&+(f^{\dagger}_{\mathbf{k}\uparrow}d_{\mathbf{q}\uparrow}-f^{\dagger}_{\mathbf{k}\downarrow}d_{\mathbf{q}\downarrow})]+S^{+}_{i}(d^{\dagger}_{\mathbf{k}\downarrow}f_{\mathbf{q}\uparrow}+f^{\dagger}_{\mathbf{k}\downarrow}d_{\mathbf{q}\uparrow})\\&+S^{-}_{i}(d^{\dagger}_{\mathbf{k}\uparrow}f_{\mathbf{q}\downarrow}+f^{\dagger}_{\mathbf{k}\downarrow}d_{\mathbf{q}\uparrow})\}\end{aligned} \quad (8)$$

describes the assisted tunneling processes through the scattering of the tunneling electrons with the localized moments[13] where $S^{x,y,z}_{i}=\Sigma_{\alpha\beta}c^{\dagger}_{i\alpha}\sigma^{\alpha\beta}_{x,y,z}c_{i\beta}$ ($\sigma_{x,y,z}$ denote the Pauli matrices) represent the moments of localized states. As is well known, this term can result in spin-flip scattering processes, in which the spin projection of one tunneling electron increases and that of one localized electron decreases, or vice versa. The last two terms are given by

$$H_4=\sum_{i\neq j}\sum_{\mathbf{kq}}\sum_{\sigma\sigma'}\{T^{(4)}_{ij\mathbf{kq}}d^{\dagger}_{\mathbf{k}\sigma}c^{\dagger}_{i\sigma'}c_{j\sigma'}f_{\mathbf{q}\sigma}+\text{H.c.}\}, \quad (9)$$

$$H_5=\sum_{i\neq j}\sum_{\mathbf{kq}}\sum_{\sigma\sigma'}\{T^{(5)}_{ij\mathbf{kq}}d^{\dagger}_{\mathbf{k}\sigma}c^{\dagger}_{i\sigma'}c_{j\sigma}f_{\mathbf{q}\sigma'}+\text{H.c.}\}. \quad (10)$$

They describe the scattering processes where one tunneling electron transfer from one FM side to the other accompanied by the hoping of one localized electron from one site to another, the difference between them is analogous to that between the direct Coulomb interaction and the exchange one.

As a simple approximation, we treat H_4 and H_5 with mean-field theory, that is to say, we replace $c^{\dagger}_{i\sigma}c_{i\sigma'}$, with their mean-field values: $\langle c^{\dagger}_{i\sigma}c_{i\sigma'}\rangle=t_{ij}\delta_{\sigma\sigma'}$. Here, we have not taken into account the polarization effect of the barrier by the magnetic electrodes because Mössbauer spectroscopy indicates that the barrier is nonmagnetic.[8] Thus, one gets

$$H_4=\sum_{\mathbf{kq}}\sum_{\sigma}\sum_{i\neq j}\{\tilde{T}^{(4)}_{ij\mathbf{kq}}d^{\dagger}_{\mathbf{k}\sigma}f_{\mathbf{q}\sigma}+\text{H.c.}\}, \quad (11)$$

$$H_5=\sum_{\mathbf{kq}}\sum_{\sigma}\sum_{i\neq j}\{\tilde{T}^{(5)}_{ij\mathbf{kq}}d^{\dagger}_{\mathbf{k}\sigma}f_{\mathbf{q}\sigma}+\text{H.c.}\}, \quad (12)$$

where $\tilde{T}^{(4)}_{ij\mathbf{kq}}=2t_{ij}T^{(4)}_{ij\mathbf{kq}}$ and $\tilde{T}^{(5)}_{ij\mathbf{kq}}=t_{ij}T^{(5)}_{ij\mathbf{kq}}$.

Now, we turn to analyze the attenuation behaviors of the tunneling matrix elements $T^{(1)}_{\mathbf{kq}}$, $T^{(3)}_{i\mathbf{kq}}$, $\tilde{T}^{(4)}_{ij\mathbf{kq}}$, and $\tilde{T}^{(5)}_{ij\mathbf{kq}}$ with the thickness of the barrier:

$$T^{(1)}_{\mathbf{kq}}=\int d\mathbf{r}\phi^{\dagger}_{l\mathbf{k}}(\mathbf{r})\left[\frac{\mathbf{p}^2}{2m}+u(\mathbf{r})\right]\phi_{r\mathbf{q}}(\mathbf{r}), \quad (13)$$

$$\begin{aligned}T^{(3)}_{i\mathbf{kq}}=&\int\int d\mathbf{r}_1 d\mathbf{r}_2\phi^{\dagger}_{l\mathbf{k}}(\mathbf{r}_1)w^{\dagger}(\mathbf{r}_2-\mathbf{R}_i)v(\mathbf{r}_1-\mathbf{r}_2)\\&\times\phi_{r\mathbf{q}}(\mathbf{r}_2)w(\mathbf{r}_1-\mathbf{R}_i),\end{aligned} \quad (14)$$

$$\begin{aligned}\tilde{T}^{(4)}_{ij\mathbf{kq}}=&2t_{ij}\int\int d\mathbf{r}_1 d\mathbf{r}_2\phi^{\dagger}_{l\mathbf{k}}(\mathbf{r}_1)w^{\dagger}(\mathbf{r}_2-\mathbf{R}_i)v(\mathbf{r}_1-\mathbf{r}_2)\\&\times\phi_{r\mathbf{q}}(\mathbf{r}_1)w(\mathbf{r}_2-\mathbf{R}_j),\end{aligned} \quad (15)$$

$$\begin{aligned}\tilde{T}^{(5)}_{ij\mathbf{kq}}=&t_{ij}\int\int d\mathbf{r}_1 d\mathbf{r}_2\phi^{\dagger}_{l\mathbf{k}}(\mathbf{r}_1)w^{\dagger}(\mathbf{r}_2-\mathbf{R}_i)v(\mathbf{r}_1-\mathbf{r}_2)\\&\times\phi_{r\mathbf{q}}(\mathbf{r}_2)w(\mathbf{r}_1-\mathbf{R}_j).\end{aligned} \quad (16)$$

They are evidently determined by the wave functions $\phi_{l\mathbf{k}}(\mathbf{r})$, $\phi_{r\mathbf{q}}(\mathbf{r})$, and $w(\mathbf{r}-\mathbf{R}_i)$. As is well known, $\phi_{l\mathbf{k}}(\mathbf{r})$ and $\phi_{r\mathbf{q}}(\mathbf{r})$, respectively, attenuate as $e^{-\kappa x}$ and $e^{-\kappa(t-x)}$ ($x\leqslant t$, x along the direction of the junction) in the barrier region[13] where t is the thickness of the barrier and κ the decay constant which is determined by the height U of the potential in the barrier region and decreases with the decrease of U, and $w(\mathbf{r}-\mathbf{R}_i)$ attenuates as $e^{-\alpha|\mathbf{r}-\mathbf{R}_i|}$ where α is the localization coefficient of the amorphous barrier (α^{-1} is the localization length). With those one can easily find from Eq. (13) to Eq. (16)

$$T^{(1)}_{\mathbf{kq}}\propto e^{-\kappa t}, \quad (17)$$

$$T^{(3)}_{i\mathbf{kq}}\propto e^{-(1/2)(\kappa+\alpha)t}, \quad (18)$$

$$\tilde{T}^{(4)}_{ij\mathbf{kq}}\propto e^{-(\kappa+2\alpha)t}, \quad (19)$$

$$\tilde{T}^{(5)}_{ij\mathbf{kq}}\propto e^{-\alpha t}, \quad (20)$$

in obtaining $\tilde{T}^{(4)}_{ij\mathbf{kq}}$ and $\tilde{T}^{(5)}_{ij\mathbf{kq}}$, we have used the fact that the main contributions to H_4 and H_5 come from the localized states near the two faces of the barrier. It is worthy of noting that $\tilde{T}^{(4)}_{ij\mathbf{kq}}$ attenuates so fast that H_4 can play a role only in the case of a very thin barrier. Now that we mainly concern the attenuation behavior of the exchange coupling in the case of quite a thick barrier, it is rational to neglect H_4 hereafter, so we arrive at our working Hamiltonian

$$H=H_0+H_1+H_3+H_5, \quad (21)$$

where H_0 describes the two FM electrodes, H_1 and H_5 represent direct and assisted non-spin-flip tunneling, respectively, and H_3 represents assisted spin-flip tunneling.

Let us suppose that the spin quantization axes of the two FM electrodes differ by θ along the y direction and that the spin vectors in the tunneling Hamiltonians H_1, H_3, and H_5 are all projected with respect to the axis of the left FM electrode, Therefore, the destruction operator $f_{\mathbf{q}\lambda}$ in H_1, H_3, and H_5 should transform as

$$f_{\mathbf{q}\lambda}=U^{\lambda s}(\theta)f_{\mathbf{q}s}, \quad (22)$$

where

$$U(\theta)=e^{(i/2)\sigma_y\theta}. \quad (23)$$

On the left-hand side of Eq. (22), the spin vector is projected with respect to the spin quantization axis of the left FM electrode, and on the right-hand side of Eq. (22), the spin vector is projected with respect to the spin quantization axis of the right FM electrode. With Eq. (22) the Hamiltonian (21) can be rewritten as

$$H=\sum_{\mathbf{k}\lambda}\epsilon_{\mathbf{k}\lambda}d^{\dagger}_{\mathbf{k}\lambda}d_{\mathbf{k}\lambda}+\sum_{\mathbf{q}s}\zeta_{\mathbf{q}s}f^{\dagger}_{\mathbf{q}s}f_{\mathbf{q}s}$$
$$+\sum_{\mathbf{kq}}\sum_{\lambda s}[T^{(1)}_{\mathbf{kq}}U^{\lambda s}(\theta)d^{\dagger}_{\mathbf{k}\lambda}f_{\mathbf{q}s}+\text{H.c.}]$$
$$-\sum_{\mathbf{kq}}\sum_{\lambda\nu s}\sum_{i}[T^{(3)}_{i\mathbf{kq}}\vec{S}_i\cdot\vec{\sigma}^{\lambda\nu}U^{\nu s}(\theta)d^{\dagger}_{\mathbf{k}\lambda}f_{\mathbf{q}s}+\text{H.c.}]$$
$$+\sum_{\mathbf{kq}}\sum_{\lambda s}\sum_{ij}[\tilde{T}^{(5)}_{ij\mathbf{kq}}U^{\lambda s}(\theta)d^{\dagger}_{\mathbf{k}\lambda}f_{\mathbf{q}s}+\text{H.c.}]. \quad (24)$$

What faces us now is to calculate, from the Hamiltonian (24), the exchange coupling which is contained in the whole interaction between the two FM electrodes. The whole interaction energy $E_{\text{in}}(\theta)$ reads

$$E_{\text{in}}(\theta)=\langle H_1\rangle+\langle H_3\rangle+\langle H_5\rangle. \quad (25)$$

Treating $H_1+H_3+H_5$ as a perturbation to H_0, expanding $E_{\text{in}}(\theta)$ to the second order of the perturbation and averaging it with respect to the randomness of the localized spins, we obtain

$$E_{\text{in}}(\theta)=\left\{\frac{1}{2}\left|A(t)+C(t)\right|^2+\frac{3}{8}\left|B(t)\right|^2\right\}\sum_{\sigma\sigma'}\chi_{\sigma\sigma'}$$
$$+\left\{\frac{1}{2}\left|A(t)+C(t)\right|^2-\frac{1}{8}\left|B(t)\right|^2\right\}$$
$$\times\sum_{\sigma\sigma'}\sigma\sigma'\chi_{\sigma\sigma'}\cos\theta, \quad (26)$$

where

$$A(t)=T^{(1)}_{\mathbf{kq}}=A_0e^{-\kappa t}, \quad (27)$$

$$|B(t)|^2=\sum_i|T^{(3)}_{i\mathbf{kq}}|^2=|B_0|^2e^{-(\kappa+\alpha)t}, \quad (28)$$

$$C(t)=\sum_{ij}\tilde{T}^{(5)}_{ij\mathbf{kq}}=C_0e^{-\alpha t}, \quad (29)$$

$$\chi_{\sigma\sigma'}=\sum_{\mathbf{kq}}\frac{f(\epsilon_{\mathbf{k}\sigma})-f(\zeta_{\mathbf{q}\sigma'})}{\epsilon_{\mathbf{k}\sigma}-\zeta_{\mathbf{q}\sigma'}}, \quad (30)$$

where the moment dependencies of the tunneling matrix elements are neglected and $f(\omega)$ is the Fermi function. We note that the minus sign before $|B(t)|^2/8$ in the second brace pair of Eq. (26) arises from the spin-flip scattering between the tunneling electrons and the localized states in the amorphous-semiconducting barrier.

Obviously, the first term in Eq. (26) has nothing to do with the exchange coupling because it is independent of θ, the angle between the magnetization axes of the two FM electrodes. The second term is a function of θ, and has the same form as a Heisenberg exchange energy, it is this term that represents the exchange interaction between the two FM electrodes. In accordance with the experiments, the exchange coupling strength J can be defined as

$$J=\tfrac{1}{2}\{E_{\text{in}}(0)-E_{\text{in}}(\pi)\}=\{\tfrac{1}{2}|A(t)+C(t)|^2$$
$$-\tfrac{1}{8}|B(t)|^2\}\sum_{\sigma\sigma'}\sigma\sigma'\chi_{\sigma\sigma'}. \quad (31)$$

Equation (31) indicates that J is the times of the two terms, the one in the braces and the one following the σ, the former, as a function of the thickness of the barrier t, originates from the tunneling matrix elements so that it reflects the effects of the intrinsic properties of the barrier on the coupling, the latter results from both of the energy bands of the left and right FM electrodes so that it reflects the effects of the intrinsic properties of the electrodes on the coupling.

According to the definition, the two FM electrodes are antiferromagnetic coupled when $J>0$, and ferromagnetic coupled when $J<0$. The sign of J is determined by the cooperating result of the two terms on the right-hand side of Eq. (31). In order to analyze the sign of J in detail, we assume, for simplicity, the two FM electrodes are made of the same material such that the dispersion relations of $\epsilon_{\mathbf{k}\sigma}$ and $\zeta_{\mathbf{q}\sigma}$ are the same. Under those considerations, one has

$$\chi_{\sigma\sigma'}=\int\int d\epsilon\,d\zeta g_{\sigma}(\epsilon)g_{\sigma'}(\zeta)\frac{f(\epsilon)-f(\zeta)}{\epsilon-\zeta}$$
$$=g_{\sigma}(0)g_{\sigma}{}'(0)\int\int d\epsilon\,d\zeta\frac{f(\epsilon)-f(\zeta)}{\epsilon-\zeta}, \quad (32)$$

where $g_{\sigma}(\epsilon)$ represents the density of states of the energy band with spin σ, and $g_{\sigma}(0)$ its value at the Fermi level. From Eq. (32), one can easily find

$$\sum_{\sigma\sigma'}\sigma\sigma'\chi_{\sigma\sigma'}=[g_{\uparrow}(0)-g_{\downarrow}(0)]^2\int\int d\epsilon d\zeta\frac{f(\epsilon)-f(\zeta)}{\epsilon-\zeta}\leqslant 0. \quad (33)$$

Equation (33) indicates the contribution to J from the electrodes is never greater than zero because the integral is always negative. Particularly, when $g_{\uparrow}(0)=g_{\downarrow}(0)$, $J=0$, i.e., there does not exist any exchange coupling between the two electrodes when they are paramagnetic. This term does not change its sign and value with the barrier thickness so that whether the exchange coupling oscillates depends only on $|A(t)+C(t)|^2/2-|B(t)|^2/8$. There are two contributions to this term, $-|B(t)|^2/8$ comes from the spin-flip tunneling produced by the Hamiltonian H_3, it favors antiferromagnetic coupling; $|A(t)+C(t)|^2/2$ comes from the non-spin-flip tunneling produced by the Hamiltonians H_1 and H_5, it favors ferromagnetic coupling. The net coupling is determined by the competition between the non-spin-flip tunneling and the spin-flip tunneling: in the region where the non-spin-flip tunneling dominates, i.e., $|A(t)+C(t)|^2>|B(t)|^2/4$, the net coupling is of ferromagnetic type; in the region where the spin-flip tunneling dominates, i.e., $|A(t)+C(t)|^2<|B(t)|^2/4$, the net coupling is of antiferromagnetic type.

The tunneling matrix elements $A(t)$, $B(t)$, and $C(t)$ are determined by the detailed properties of the barrier, there-

fore, in order to discuss the competition between the spin-flip tunneling and the non-spin-flip tunneling, it is necessary for us to investigate in detail which properties of the amorphous-insulating barrier influence them. Equation (27) indicates $A(t)$ is a reflection of the height of the potential in the barrier region which is, as emphasized before, proportional to the gap of the barrier, thus, the lower the gap is, the smaller the κ is.[11,12] On the other hand, from Eq. (29) we see that $C(t)$ reflects both the extent of the localization which is measured by α and the concentrations of the localized electrons and holes through the sum over i and j, $C_0 \propto \rho_e \rho_h$ where ρ_e and ρ_h are the concentration of the localized electrons and that of the localized holes, respectively. $B(t)$ reflects all the effects of the gap, localization, and concentration of the localized electrons [see Eq. (28)], $|B_0|^2 \propto \rho_e$. In a word, the gap and localization of the barrier control the attenuation behaviors of the tunneling matrix elements $A(t)$, $B(t)$, and $C(t)$, and the concentrations of the localized electrons and holes change the amplitudes of $B(t)$ and $C(t)$, but have no influence on the amplitude of $A(t)$.

For amorphous semiconductors, α can be evaluated from the density of states at the Fermi level,[12] and κ can be estimated approximately from the formula $\kappa = \sqrt{2m_e U}$ which is the result of Schrödinger equation in the barrier region (see Fig. 2), For a-Si, a-Ge, and a-SiO, $\alpha^{-1} = 3 \sim 12$ Å,[12], and $E_g = 0.8 \sim 1.3$ eV which leads to $U = 0.4$–0.65 eV and further to $\kappa^{-1} = 15$–25 Å. That means $\alpha > \kappa$ for a-Si and a-Ge, so $C(t)$ attenuates more quickly than $B(t)$, and $B(t)$ attenuates more quickly than $A(t)$. Therefore, if $B(t)$ is large enough, there will appear an antiferromagnetic region in the middle range of the barrier thickness, the ferromagnetic regions occupying the two sides of it, in other words, the exchange coupling will oscillate from ferromagnetic type to antiferromagnetic one and back to ferromagnetic one with the increasing of the barrier thickness. The antiferromagnetic region shrinks gradually with the decreasing of $B(t)$, when $B(t)$ becomes very small it will disappear so that there will exist only ferromagnetic region in the whole range of the barrier thickness. Since $|B_0|^2$ is proportional to the concentration of the localized electrons, ρ_e, in the barrier, the previous analysis means that the amorphous barrier with a high concentration of localized defects favors the occurrence of a oscillating exchange coupling. That is why the experimental observations show that the coupling is oscillatory in Fe/Si/Fe but always ferromagnetic in Fe/Ge/Fe because the concentration of the localized defects in a-Si is higher than the a-Ge.[6]

As an illustration of those interpretations, we have shown our numerical results of Eq. (31) in Figs. 3 and 4. From them one can easily see that the exchange coupling oscillates when $B(t)$ is large enough, with the decreasing of $B(t)$, the oscillatory strength gets weaker and weaker and disappears in the end such that the coupling becomes always ferromagnetic.

In summary, we have developed a tunneling model for the exchange coupling between the two FM electrodes separated by an amorphous-semiconducting barrier. The tunneling Hamiltonian consists of two kinds of processes: the spin-flip tunneling and the non-spin-flip tunneling, the non-spin-flip Hamiltonian has two pieces, one is the direct tunneling term, the other is the assisted term. The direct tunneling attenuates most slowly and is responsible for the ferromagnetic coupling in the long range of the barrier thickness, the assisted non-spin-flip tunneling attenuates most fast and is accountable for the short-range ferromagnetic coupling, the spin-flip tunneling attenuates neither fast nor slowly and is responsible for the antiferromagnetic coupling possibly emerging in the middle range. The coupling is oscillatory with the thickness of the barrier if the spin-flip tunneling is strong enough, and always ferromagnetic if the spin-flip is weak. Those interpretations are qualitatively in agreement with the experiments.

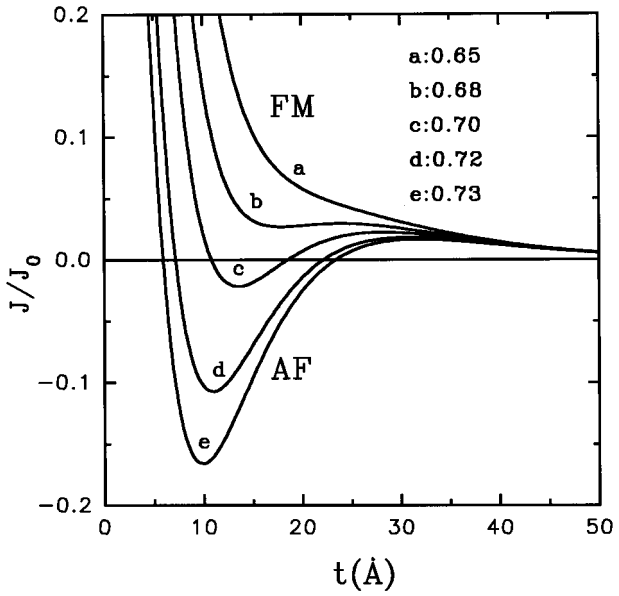

FIG. 3. The exchange coupling vs the barrier thickness. Here $J_0 = |C_0|^2 \Sigma_{\sigma\sigma'} \chi_{\sigma\sigma'}/2$, $C_0/A_0 = 3.0$, $\kappa^{-1} = 8$ Å, $\alpha^{-1} = 20$ Å, and the curves a, b, c, d, and e correspond to $B_0/A_0 = 0.65$, 0.68, 0.70, 0.72, and 0.73.

The above discussions are restricted to the zero temperature. As for finite temperatures, the increase of the coupling with temperature becomes an important characteristic of the amorphous semiconducting barrier. It reminds us of the con-

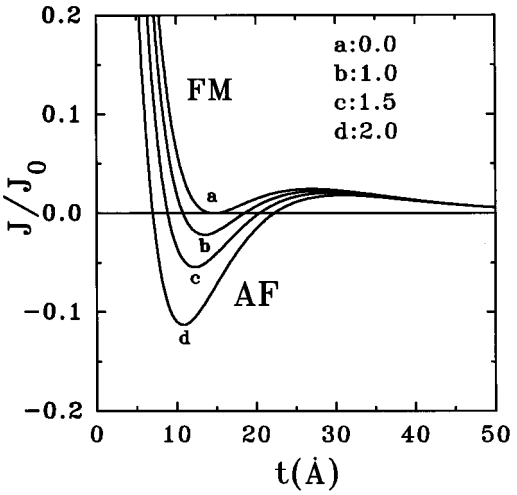

FIG. 4. The exchange coupling vs the barrier thickness. Here $J_0 = |C_0|^2 \Sigma_{\sigma\sigma'} \chi_{\sigma\sigma'}/2$, $C_0/A_0 = -2.0$, $\kappa^{-1} = 8$ Å, $\alpha^{-1} = 20$ Å, and the curves a, b, c, and d correspond to $B_0/A_0 = 0.0$, 1.0, 1.5, and 2.0.

ductivity present in the amorphous semiconductors (Mott's $T^{1/4}$ law) and the phonon-assisted tunneling conductance of the junction with an insulating barrier, they both increase with the increasing of temperature, too. The main physical reason for them is considered to be the electron-phonon interaction which leads to phonon-assisted hopping of the electrons in the localized states of the amorphous semiconductor and phonon-assisted tunneling of the tunneling electrons, respectively. Those jointly mean that the electron-phonon interaction will play a central role in an amorphous tunneling barrier. Therefore, we believe it is the electron-phonon interaction that is accountable for the increase of the exchange coupling across an amorphous spacer with increasing temperature. The corresponding finite-temperature theory containing the effects of the phonons in the amorphous spacers is being under working and will be published elsewhere.

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