Comment on "Exchange Coupling in Magnetic Multilayers: A Quantum-Size Effect"

In a recent Letter, Muñoz and Pérez-Díaz (MPD) [1] have considered the problem of interlayer exchange coupling between two ferromagnetic layers separated by a nonmagnetic spacer of thickness D. In the case of a spacer potential well of depth V, they argue that, in addition to the usual coupling oscillations (versus spacer thickness) of period π/k_F, the quantum-well states give rise to oscillations of period π/k_0 where $k_0 \equiv \sqrt{2mV}/\hbar$. Previously, a Letter presenting essentially the same argument has been published by Jones and Hanna (JH) [2]. Both papers are based on the perturbative Ruderman-Kittel-Kasuya-Yosida (RKKY) theory. In a Comment on the JH Letter, it was shown by using an exact analytic approach that the claimed oscillations of period π/k_0 are spurious [3]. In the present Comment, first we show that the expression obtained by MPD yields erroneous results, even in the case of vanishing well depth, then we discuss the origin of the spurious structure due to the bound states.

To see that the results of MPD are erroneous in the limit of vanishing well depth, consider first the well known RKKY interlayer coupling for a flat potential [4],

$$J_{\mathrm{RKKY}} \sim \frac{2k_F D\cos(2k_F D) - \sin(2k_F D)}{4D^2} - k_F^2 \int_{2k_F D}^{+\infty} \frac{\sin x}{x}\, dx \,. \qquad (1)$$

According to MPD, the expression of the RKKY coupling across the potential well is given by (Eq. (7) of [1])

$$J_{\mathrm{MPD}} \sim \mathrm{Im} \int_0^{k_F} (k_F^2 - k^2)\, \frac{t^2(k) e^{2ikD}}{k}\, dk \,, \qquad (2)$$

where $t(k)$ is the transmission coefficient through the potential well. The case of vanishing well depth is obtained by setting $t(k) = 1$ in Eq. (2), which immediately yields

$$J_{\mathrm{MPD}} \sim J_{\mathrm{RKKY}} + k_F^2 \frac{\pi}{2} \,. \qquad (3)$$

The last term in the right-hand side of Eq. (3) gives a finite coupling at infinite spacer thickness, which is obviously incorrect. This spurious extra term is reminiscent of a similar error made by Kittel in his original treatment of the RKKY interaction in one dimension [5], which he subsequently corrected in an Erratum, and which has been discussed in detail in Ref. [4].

Recently, a formulation of the problem of interlayer coupling in terms of reflection coefficients at the interfaces (RCI) has been proposed [6], which allows a nonperturbative calculation of the coupling. This approach has been applied to the problem discussed by MPD; in the case of vanishing well depth, it yields [3]

$$J_{\mathrm{RCI}} \sim \mathrm{Im} \int_{0+i0^+}^{k_F+i0^+} (k_F^2 - k^2)\, \frac{e^{2ikD}}{k}\, dk \,; \qquad (4)$$

the only difference with the expression of MPD, Eq. (2) with $t(k) = 1$, is that the integration is not performed on the real axis, but slightly above the real axis. As one can check easily, the correct result, Eq. (1), is obtained. The expression of MPD, Eq. (2), yields a spurious term because their integration path runs through the pole at $k = 0$, which is avoided in Eq. (4).

MPD calculate the exchange coupling using distorted wave perturbation theory. For distorted waves, the distribution of states is not uniform in reciprocal space as it is for plane waves, and the sum over intermediate states cannot simply be replaced by an integration over wave vector. Bound states, which cannot be indexed by a wave vector, are the most dramatic example. These states, which must be included, are neglected by MPD. The changes in the densities of states in the continuum, due to resonances, are also neglected. This neglect leads to the spurious discontinuities as a function of thickness whenever a new bound state is introduced.

In distorted wave perturbation theory, particular care is needed in treating the states close to the threshold energy. As the thickness of the well increases, resonances in the continuum sink lower in energy and sharpen. When their energy reaches the threshold energy, they become bound states. When distorted wave perturbation theory is done correctly, changes due to the resonances exactly cancel those from the bound states. Spurious discontinuities result if the bound states and the change in the continuum density of states are ignored as done by MPD, or if just the change in the continuum density of states is ignored as done by JH.

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