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Condensed matter physics in the 21st century: The legacy of Jacques Friedel

The longevity of Jacques Friedel's model of the virtual bound state

La longévité du modèle d'état lié virtuel de Jacques Friedel

Peter M. Levy [a,*], Albert Fert [b,c]

[a] *Department of Physics, New York University, 4 Washington Place, New York, NY 10003, USA*
[b] *Unité mixte de physique CNRS/Thales, 91767, Palaiseau, France*
[c] *Université Paris-Sud, 91405 Orsay cedex, France*

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ABSTRACT

We illustrate the continuing pertinence of Friedel's model of the virtual bound state to describe electron scattering in metals. This model has been applied to such disparate studies as the chirality of spin interactions in metals, and the spin Hall effect caused by scattering from impurities with spin–orbit coupling.

RÉSUMÉ

Nous illustrons la pertinence toujours actuelle du modèle de l'état lié de Friedel pour décrire la diffusion des électrons dans les métaux. Ce modèle a été appliqué à des problèmes aussi différentes que la chiralité des interactions de spin dans les métaux ou l'effet Hall de spin causé par la diffusion d'impuretés avec couplage spin–orbite.

1. Introduction

Many phenomena in solids involve the scattering of conduction electrons by substitutional impurities. During his doctoral thesis work with Neville Mott, Jacques Friedel studied the distribution of electrons around impurities in metals, and developed a method of virtual bound states [vbs] to describe the scattering of conduction electrons by the localized states of impurities [1]. It is based on describing scattering by a central impurity in terms of phase shifts of the incoming wave, and has been applied to a myriad of problems. The hybridization of the local states with the conduction electron states produces a broadening in the energy of the states; this is known as a vbs. When the energy of the localized state is close to the Fermi level, they affect electron transport. In the immediate vicinity of the impurity, the wave function is dominated by that of the local state; outside a range of the order of 1 nm, the wave function is that of a phase-shifted plane wave. These phase shifts are the signature of impurity scattering and affect electron transport in metals.

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[*] Corresponding author.
E-mail address: levy@nyu.edu (P.M. Levy).

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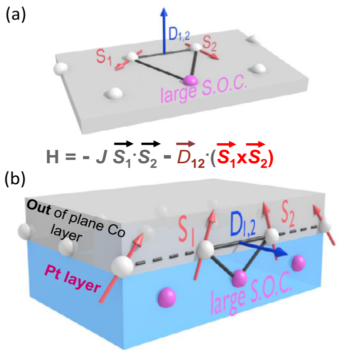

Fig. 1. (a) Triangular geometry that gives rise to DMI between the two atomic spins neighboring a nonmagnetic atom with large spin–orbit interaction. (b) A pair of atomic spins at the interface of a magnetic film with a metallic layer with large spin–orbit coupling in a noncentrosymmetric environment. Both figures are taken from Ref. [13].

To underscore the current use of Friedel's concept of a vbs, we focus on two phenomena: the spin Hall effect [SHE] due to scattering by impurities, and the chirality of exchange interactions between spins in disordered alloys or at the interface of magnetic films. Both phenomena rely on spin–orbit coupling [SOC]; hence a vbs model with orbit-dependent phase shifts is the appropriate method to describe spin–orbit split localized states in metals. The SHE induced by impurities relies on the phase shifts induced by nonmagnetic impurities that have spin–orbit coupled orbitals, while the chirality of indirect exchange arises when the phase shifted vbs's interact with neighboring local moments. The chirality arises from the character of the vbs close, of the order of 1–2 nm, to the local moments sensed at a distance through phase-shifted waves.

In the past five years there has been a renewed interest in the spin Hall effect as a source for converting charge into spin currents, e.g., the works by Mertig et al. [2], Maekawa et al. [3], as well as ours [4]. In all of these treatments, the scattering of conduction electrons by impurities that produce this effect is related to phase shifts that are determined from ab-initio calculations. In another vein, we studied [5] the anisotropy induced by ternary impurities, e.g., Pt, on the coupling between spins, Mn impurities, in metals such as Cu. In this work we first determined the scattering of conduction electrons by the impurities with strong spin–orbit coupling; subsequently the distorted waves emanating from the impurity interact with local moments at some distance from the center. The indirect coupling of two such moments interacting with the distorted waves is anisotropic; spin–orbit coupling makes coupling sensitive to the coordinates of the moments relative to the central scatterer. In the following, we review the role of phase shift analyses in conjunction with virtual bound states in determining these effects. This picture, that was first worked out for disordered alloys with low local symmetry, has been extended to situations in which inversion symmetry is broken for spins at the interface of a magnetic film. The resulting chiral interactions of the Dzyaloshinsky–Moriya type (DMI) are at the origin of the magnetic skyrmions in thin magnetic films deposited on a metal with large SOC [6].

Our article is limited to the application of the vbs model to the calculation of the SHE and the DMI. However, we point out that other concepts introduced by Friedel a long time ago are fashionable today, e.g., in the extensions of the Friedel oscillations concept to the situation where Rashba surface interactions give rise to skyrmionic spin oscillations [7].

2. Dzyaloshinsky–Moriya exchange interaction (DMI)

2.1. DMI in disordered magnetic alloys (spin glasses)

The interaction between local moments in metals, e.g., in CuMn spin glasses, is usually of the Ruderman–Kittel–Kasuya–Yosida (RKKY) type and isotropic, i.e., of the form $S_1 \cdot S_2$; however, it was found that the addition of nonmagnetic impurities with strong spin–orbit coupling (Au, Pt) sharply increases the anisotropy field that maintains the remanent magnetization in the direction of the initial applied field. In other words, by adding ternary impurities such as Pt, the local moments are harder to rotate, i.e. the anisotropic energy increases. At first, it was thought that the interaction between moments develop a pseudo dipole–dipole anisotropy. The surprising discovery was that it was primarily of the Dzyaloshinsky–Moriya (DM) form $D \cdot S_1 \times S_2$. The method used by us to find this relied on Friedel's description of localized states in metals, i.e., the vbs [5]; here we outline the method used.

The RKKY interaction is based on the calculation of the shift in the ground-state energy of a gas of conduction electrons interacting with two localized spins. Here we add a spin–orbit interaction on the site of a neighboring nonmagnetic impurity at $R = 0$ (see Fig. 1a) and therefore consider the following perturbing potential of the electron gas:

$$V = -\Gamma\delta(r - R_A)s \cdot S_A - \Gamma'\delta(r - R_B)s \cdot S_B + \lambda(r)l \cdot s \qquad (1)$$

On the site of a nonmagnetic transition-metal impurity, the spin–orbit coupling of a conduction electron is considerably enhanced because the admixture of the impurity d states into the conduction band allows the conduction electrons to

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