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

Jacques Friedel and the physics of metals and alloys

Jacques Friedel et la théorie des métaux et alliages

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ABSTRACT

This is an introduction to the theoretical physics of metals for students and physicists from other specialities. Certain simple consequences of the Fermi statistics in pure metals are first addressed, namely the Peierls distortion, Kohn anomalies and the Labbé–Friedel distortion. Then the physics of dilute alloys is discussed. The analogy with nuclear collisions was a fruitful starting point, which suggested one should analyze the effects of impurities in terms of a scattering problem with the introduction of phase shifts. Starting from these concepts, Friedel derived a theory of the resistivity of alloys, and a celebrated sum rule relating the phase shifts at the Fermi level to the number of electrons in the impurity, which turned out to play a prominent role later in the context of correlated impurities, as for instance in the Kondo effect. Friedel oscillations are also an important result, related to incommensurate magnetic structures. It is shown how they can be derived in various ways: from collision theory, perturbation theory, self-consistent approximations and Green's function methods. While collision theory does not permit to take the crystal structure into account, which is responsible for electronic bands, those effects can be included in other descriptions, using for instance the tight binding approximation.

RÉSUMÉ

Cet article est une introduction à la théorie électronique des métaux. Il s'adresse aux étudiants et aux physiciens non spécialistes. On commence par décrire certaines conséquences simples de la statistique de Fermi–Dirac dans les métaux purs, comme la distorsion de Peierls, les anomalies de Kohn et la distorsion de Labbé–Friedel. On discute ensuite la physique des alliages dilués. L'analogie avec le problème des collisions nucléaires fut un point de départ fructueux, qui amena à considérer l'effet des impuretés comme un problème de diffusion, dans lequel apparaissent les déphasages de l'onde électronique diffusée. Friedel élabora ainsi une théorie de la résistivité des alliages, et établit une règle de somme qui relie les déphasages au niveau de Fermi à la charge de l'impureté. Cette règle de somme joua plus tard un rôle essentiel dans le cas d'électrons fortement corrélés, notamment dans l'effet Kondo. Une autre découverte importante fut celle des oscillations de Friedel, responsables par exemple de la formation

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de structures magnétiques incommensurables. On montre comment elles peuvent être déduites de diverses méthodes : de la théorie des collisions, de la théorie des perturbations, d'approximations self-consistentes ou de la méthode des fonctions de Green. Si la théorie des collisions ne tient pas compte de la structure électronique, et par conséquent de la structure de bandes, ces effets peuvent facilement être inclus dans d'autres théories, par exemple en faisant appel à l'approximation des liaisons fortes.

1. Introduction

The language of physicists evolves. In this issue of the *C. R. Physique* devoted to Jacques Friedel, articles by physicists of various generations and various sub-specialities coexist, and their language is different. This makes communication with non-specialists and students difficult. The aim of the present introduction is to bridge the gap between experts and newcomers, to allow students to read old textbooks, which may be very useful because they were written by those who discovered the phenomena and often understand them better because they remember the difficulties they met, the mistakes which should be avoided, the approximations that failed and those that succeeded. We try to present a synthetic view of a few essential concepts of metal physics.

2. Simple mechanisms in pure metals

The physics of metals, where electrons are not localized, but itinerant, is a difficult matter. In the middle of the twentieth century, a few physicists tried to define basic concepts that can bring a better understanding. Among them, Jacques Friedel's part was particularly important.

The task was facilitated by previous discoveries, for instance the *Jahn–Teller distortion*, discovered in 1937 [1], which will now be briefly recalled [2]. Assume a highly symmetric system (a complex or an impurity in a crystal) where an electronic state is (for instance twice) degenerate and occupied by a single electron. The Jahn–Teller theorem states that this high symmetry state is unstable and distorts. The reason is that a weak distortion (or any small perturbation) always splits the degenerate levels into one which is at higher energy and one which is at lower energy (Fig. 1a). The electron goes into the lowest state, and thus the energy is lowered by the distortion. The Jahn–Teller distortion occurs whenever an electronic state has a n-fold degeneracy and is occupied by less than n electrons. An example (Fig. 1b) is given by an octahedral complex in which the central ion has a single valence electron on a p-shell. The electron has to choose between 3p orbitals that are directed along the three axes of the octahedron. If it chooses for instance the z axis, the distance a between the ligands on this axis is different from the distance b between the ligands on axes y and z.

The Jahn–Teller distortion occurs in small complexes or in insulators containing impurities, but similar effects occur in metals because electronic states just above and just below the Fermi surface are *nearly* degenerate. An example is the *Peierls distortion* [3–5]. It is an instability of a one-dimensional conductor formed by electrons interacting with regularly spaced ions. The ions lower the electronic energy if they modulate their distance with a period π/k_F, where k_F is the Fermi wave vector of the electron gas. The reason is the following: the distortion mixes electronic states of wave vectors k and $k-2k_F$. If k is very slightly larger than k_F, then $k-2k_F$ is very slightly larger than $-k_F$ and the corresponding energies $\epsilon(k)$ and $\epsilon(k-2k_F)$ are almost equal. The distortion lowers the lower energy and increases the higher level, but since there is no electron on this level, the total electronic energy is lowered.

The Peierls distortion (Fig. 2) is a property of one-dimensional conductors (which make them insulating or semiconducting!). But similar effects occur in certain three-dimensional metals. It has even been suggested [5] that the crystal structure of many covalent materials may be considered as resulting from a Peierls distortion of a fictitious metal. In subsection 2.2, a distortion particular to certain three-dimensional crystal structures will be addressed.

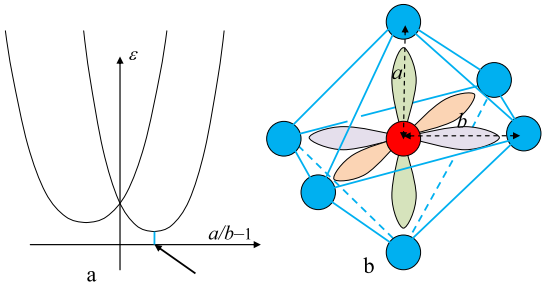

Fig. 1. The Jahn–Teller effect. a) Energy of an electron as a function of the distortion a/b of the surrounding. If there are two (or more) degenerate states in the highly symmetric state, a slight distortion increases one of the energies and lowers the other one(s). If there is a single electron, its energy is therefore lowered, b) Example of an ion in an octahedral environment with a partly occupied p shell.