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POSITRON ANNIHILATION IN SOLIDS

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Abstract : We present the technique of positron annihilation. We focus our attention to the study of the electron momentum distribution in solids. We show how the Fermi surface of metallic materials can be studied and we emphasize some recent developments started up to investigate many-body correlations effects in transition metals and compounds.

1. Introduction

Positron annihilation is a widely used tool in solid state physics [1]. Let us mention the study of structural defects, phase transitions, radiation damage, electronic surface states, positronium formation, positron dynamics, positron channeling and electron momentum distribution by angular correlations. We will restrict the scope of this paper to this last field which has known a large evolution during the last few years.

Until some years ago, the study of the electronic properties with positron annihilation was rather limited. The design of experiments was such that measurements gave only one dimensional profiles of the electron momentum distribution. The development of two dimensional position sensitive gamma rays detectors has given a new impulse to this method and the results which are actually obtained contain a much larger amount of information.

These machines yields $N(p_x, p_y)$, the 2D-angular correlations of the positron annihilation radiation, which is given by

$$N(p_x, p_y) = \int_{-\infty}^{+\infty} \rho(\vec{p})\, dp_z \tag{1}$$

where $\rho(\vec{p})$ is the two-photon momentum distribution [2]. We will discuss how this quantity relates to the electron momentum distribution in the next section.

At Geneva, M. Peter and his group have been one of the pioneers in the development of the 2D-angular correlation technique. They have developed the first spectrometer using high density proportional chambers [3]. These detectors [4] are specially well designed for the detection of the small angular deviation from the straight line (a few mrad) of the two gamma rays emitted when a positron annihilates with one electron of the target material. The good spatial resolution of high density proportional chambers yields a high angular resolution as well as a good counting rate.

2. Determination of the Fermi surface

With the angular correlation technique, the observable quantity is the two photon momentum density of the positron annihilation radiation. It is given by:

$$\rho^{2\gamma}(\vec{p}) = \sum_{\vec{k},\ell} \varepsilon(\vec{p},\ell)\, n(\vec{k},\ell)\, \left|\int e^{-i\vec{p}\vec{r}}\psi_+(\vec{r})\psi_{\vec{k},\ell}(\vec{r})\, d^3r\right|^2 \tag{2}$$

where $\psi_{\vec{k},\ell}(\vec{r})$ and $\psi_+(\vec{r})$ are respectively the electron and positron wave functions. $n(\vec{k},\ell)$ is the occupation number of the state $\vec{k}$ of the band ℓ and $\varepsilon(\vec{p},\ell)$ is a function (known or not) included to describe the many-body effects.

If we neglect $\varepsilon(\vec{p},\ell)$ for a moment, the two photon-momentum density can be expressed by

$$\rho^{2\gamma}(\vec{p}) = \sum_{\vec{k},\ell} n(\vec{k},\ell) \sum_{\vec{G}} \delta(\vec{p}-\vec{k}-\vec{G})\, |A_{\vec{G}}(\vec{k},\ell)|^2 \tag{3}$$

where

$$A_{\vec{G}}(\vec{k},\ell) = \int_{\text{cell}} e^{-i(\vec{k}+\vec{G})\vec{r}}\psi_+(\vec{r})\psi_{\vec{k},\ell}(\vec{r})\, d^3r \tag{4}$$

The delta function in (3) shows that each $\vec{k}$ state gives contributions to momentum $\vec{k}+\vec{G}$, $\vec{G}$ being the reciprocal lattice vectors. By reducing this $\vec{p}$-space distribution into the first Brillouin zone one obtains finally the occupation number $n(\vec{k},\ell)$ if the positron wave function can be described by a constant. In reality this condition is nearly fulfilled: the positron is thermalized at the time of its annihilation and it lies in the lowest state ($\vec{k}=0$) of an s band. Therefore, the Fermi surface can be determined if these approximations hold: the correlation effects are not too important and the positron wave function is flat. Fortunately, these approximations usually hold and the determination of the Fermi surface from two dimensional angular correlation distributions (equation 1) restricts itself to the problem of constructing an object from its projections. Many methods exist to do this. We are using the back-projection technique developed for the tomography.

We show in figure 1 the Fermi surface of V_3Si [5] determined by this method. This compound belongs to the A15 family which includes most of the good superconductors. The Fermi surface determined by positron annihilation is in good agreement with the one obtained by calculating the band structure of this compound. V_3Si is a typical example of the state of the art presently achieved in this field. It demonstrates the ability we now have to determine Fermi surfaces in alloys and compounds, whereas the traditional techniques based on the cyclotron resonance can not be used: they request magnetic fields beyond the limit of the technology. The Fermi surface of other A15 materials have also been determined [6]. In disordered alloys, very encouraging results have been obtained and it has been shown that, in system like Nb-Mo or Cu-Ni, the disorder does not blur the Fermi surface completely.

3. Study of the many-body correlations

Beyond the determination of the Fermi surface, very valuable information can be obtained about the electronic wave functions when analyzing the two-photon momentum density in the $\vec{p}$-space. The calculation of this quantity requires very accurate numerical algorithms. The positron group of M. Peter has developed, under the impulse of T. Jarlborg and A.K. Singh, a scheme taking great advantage of the Linear Muffin Tin Orbital (LMTO) [7] method. The conjunction of fine measurements and very precise calculations of the two-photon momentum density has recently opened a new field of investigations: the effects of the many-body interactions.

This field has been studied carefully by L. Oberli et al [8] in alkali metals. In these materials the situation is rather simple due to their free-

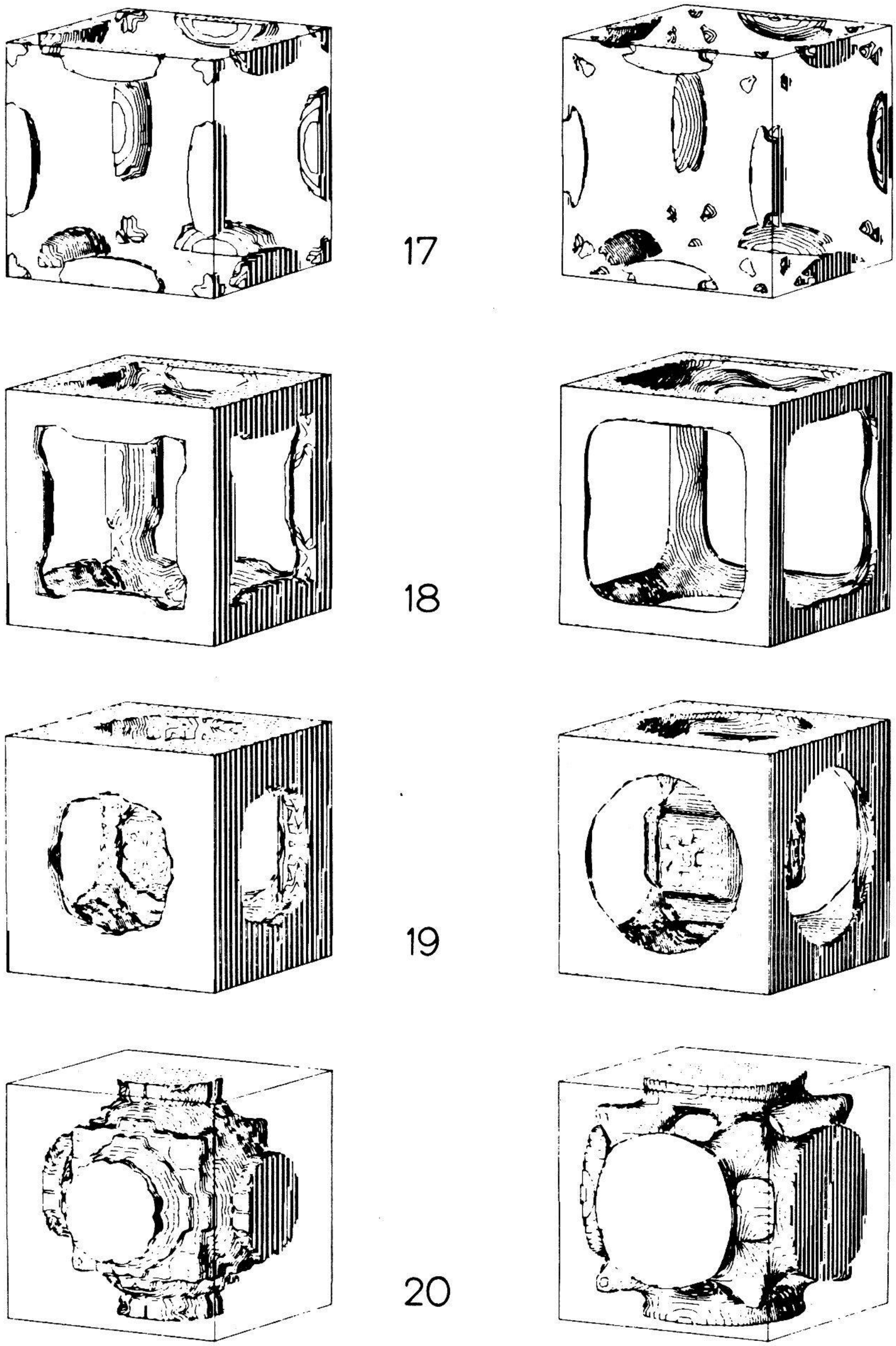

Figure 1: *The Fermi surface of the superconducting compound V_3Si. On the left, the positron annihilation result is shown while the calculated Fermi surface is pictured on the right (from reference [5])*

electron-like behavior. But even in these simple metals there is not complete accord among many-body theorists about the effects of the electron-positron interactions.

While all many-body theorists agree that the correlations will enhance the results obtained in the independant particle model by a factor $\varepsilon(p)$ well represented by $a + b(p/p_F) + c(p/p_F)^2$, where p_F is the Fermi momentum, how this enhancement factor varies with the electronic density was a controversial subject where the fine experimental results of Oberli et al [8] were able to give a clear answer.

If the correlation effects in alkali metals seems now to be correctly understood, the situation in non-simple metals is much worse. Very recently, we have found some new manifestations of these correlations effects: measurements in Ni by Walker et al [9] have revealed a new behavior, illustrated in Figure 2 [10].

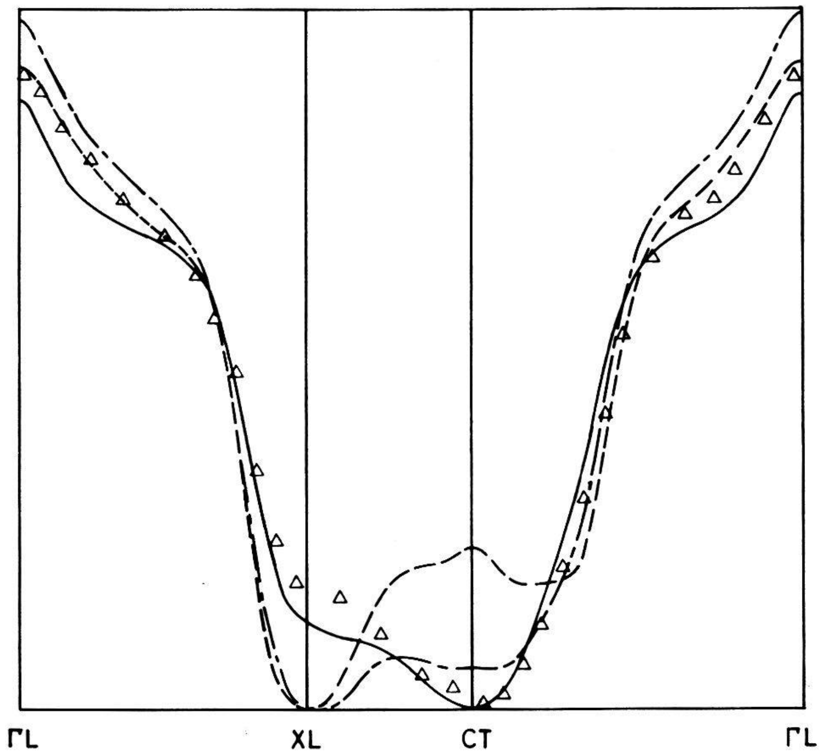

Figure 2: Some lines extracted from the two-photon momentum distribution of Ni after reduction to the $\vec{k}$-space. The triangles are the experimental points. The hashed line is the calculated Fermi surface cross-section. The chain line shows the effect of the positron wave function. But only the full line is able to reproduce all the features of the experiment; it is obtained by the phenomenological model of the many-body correlations described in the text.

We have found in Ni that the correlations can be described by a de-enhancement factor depending on the distance between the electronic energies and the Fermi energy. Our model is only phenomenological and no theory today is able to explain this new behavior. That is why we are especially happy to expose this new phenomenon for the first time at the occasion of this seminar devoted to Professor C.P. Enz. Professor Enz's career distinguished with many important contributions to the problem of theoretical physics [11]. Would it be possible that a model describing the electron-positron interactions in transition metals will be born at Geneva? Without any doubt, such a contribution of the theoretical physicists is essential in order to progress in the study of the electronic properties of solids by positron annihilation.

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