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## ELECTRON-POSITRON SCATTERING IN REAL METALS

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The purpose of the paper is to point at the importance of some detailed studies of electron-positron scattering in real metals using wave functions obtained from band structure calculations. In this work some preliminary investigations of the matrix elements of electron-positron scattering, e.g. the transitions from occupied to non-occupied states close to the Fermi surface are presented. One can observe that for  $s \rightarrow s$  transitions of the positron ( $s, p$  are orbital quantum numbers) electrons do not change their orbital quantum numbers but for  $s \rightarrow p$  transitions of the positron, electron quantum numbers change by unity.

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One of the most important quantities in the positron annihilation method of investigating metals is the momentum density distribution of electron-positron (e-p) pairs  $R(p)$ . To calculate it properly, one should take into account both the crystallic nature of e-p wave functions and the e-p interaction. A great progress has been made as concerns the theory of e-p interaction in a homogeneous electron gas (see e.g. [1]). It is much more difficult to describe this interaction in real metals. The reasons are, among others, the deviation of electron and positron functions from plane waves, the hybridization of electronic states and the unknown e-p potential in inhomogeneous systems. By now, in principle, there are two ways of solving this problem. One is to apply some final results of e-p interaction theory for a homogeneous electron gas (e.g. [2]) concerning the momentum dependent enhancement factor  $\varepsilon(p)$ . The idea of Daniuk et al. [3] was to use it locally under the appropriate integral for  $R(p)$ :

$$R(p) = \sum_{k,n} \int \exp(-ip \cdot r) \sqrt{\varepsilon_{kn}(r_s(r))} \psi_+(r) \psi_{kn}(r) dr, \quad (1)$$

where  $\varepsilon_{kn}$  is obtained from the calculations of Rubaszek and Stachowiak [2]. This approximation seems to lead to reasonable conclusions [4].

In the alternative approach to this problem called BML (Bloch-modified ladder) theory emphasis is put on the Bloch character of the one-particle wave functions (Sormann [5]). BML is a simplification of the old idea of Carbotte [6] which

in its original form was too complicated to allow for more extensive calculations. In this case the appropriate enhancement is found by solving a Bethe–Goldstone-type (BG) equation in which, unlike in the local density approximation, the potential of e–p interaction is assumed to be independent of the positron coordinates. The occupied electron and positron states are described by APW wave functions, but the excited states, however, are assumed to be plane waves (PW) and the Fermi surface is just a sphere of radius resulting from the average density of electrons. From a recent paper of Sormann and Wallner [7] in which they approximate all wave functions as superpositions of PW it results that the values of the enhancement may depend appreciably on the way of approximating the excited states (calculations made in Born approximation). The details of the effect, unfortunately, are not fully understandable. When APW functions (superpositions of PW) are used instead of single plane waves to describe excited states, one does not know clearly which effects play a role in this change, what causes that the enhancements are for one metal smaller than the corresponding ones calculated on a base of plane waves and why they are greater for the other metal. In our opinion, solving of this equation in momentum space causes that some of the mechanisms of scattering are not evident (e.g. the way the electrons and the positron change their state). Besides, the limited number of coefficients in the Fourier expansion of APW functions with respect to reciprocal-lattice vectors  $\mathbf{G}$  used in the BG equation may lead to an error for a limited number of  $\mathbf{G}$ , especially for transition metals.

In the method proposed by Boroński and Jarlborg [8] the BG equation is also used, but in real space and with a potential locally dependent on the positron position. This allows to follow some other aspects of the e–p interaction (Fig. 1). The basis set of Bloch functions for both occupied and excited states is taken from linear muffin-tin orbital calculations. However, in the paper [8] some approximations concerning calculating of matrix elements have also been made resulting in greater errors in enhancement for the region near to the ion core.

Having in mind all recent results concerning the use of more realistic electron and positron wave functions and the deficiencies of the mentioned approaches, we would like to understand some details of e–p scattering and to check how meaningful are the approximations concerning the description of occupied and excited states for different metals. As the first step we investigate here the crucial point of most calculations, namely the matrix element in the e–p scattering formulae.

If one takes the BG equation as a model formalism, the basic formula for correlated e–p wave function can be assumed as

$$\Psi_{\mathbf{k}}^j(r_+, r_-) = \phi_{\mathbf{k}}^j(r_-)\phi_0^+(r_+) + \sum_{\substack{\mathbf{k}', s \\ \alpha, \beta}} \frac{\phi_{\mathbf{k}'}^\alpha(r_-)\phi_s^{+\beta}(r_+)M_{\mathbf{k}\mathbf{k}'s}^{j\alpha\beta}}{E_{\mathbf{k}}^j - E_{\mathbf{k}'}^\alpha + E_0^+ - E_s^{+\beta}} \quad (2)$$

where

$$M_{\mathbf{k}\mathbf{k}'s}^{j\alpha\beta} = \langle \phi_{\mathbf{k}'}^\alpha(r'_-)\phi_s^{+\beta}(r'_+) | V(r'_+, r'_-) | \Psi_{\mathbf{k}}^j(r'_+, r'_-) \rangle. \quad (3)$$

The basic set of functions coming into (2) are one-particle electron Bloch functions  $\phi_{\mathbf{k}}^j(r)$  given by band structure calculations ( $j, \alpha, \beta$  are band labels), and a positron

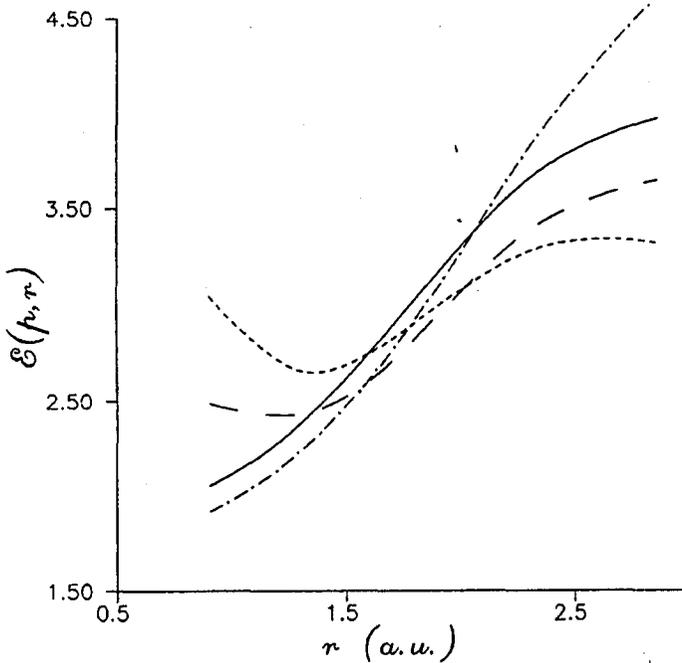


Fig. 1.  $r$ -dependent enhancement for Pd ( $p = 0.4k_F$ ) (from Ref. [8]). — electron and positron excited states are described by plane waves; ---- only electron excited states are described by plane waves; - - - - only positron excited states are described by plane waves; - - - all excited states reflect the band structure.

wave function of the type

$$\phi_s^{+\beta}(r) = \frac{1}{\sqrt{N}} u_s^\beta(r) e^{i s \cdot r}, \quad (4)$$

where  $u_s(r)$  can also be found from band structure calculations for a positron. The summation in (2) extends over all electron and positron states in the first Brillouin zone which are not occupied. The effective potential may, in general, depend on the position in the lattice.

Since the main effects of the influence of the Bloch character of wave functions should be seen already in first order of perturbation theory, in further calculations we shall replace  $\Psi_{\mathbf{k}}^j(r'_+, r'_-)$  in (3) by non-interacting functions  $\phi_{\mathbf{k}}^j(r'_-)$  and  $\phi_0^+(r'_+)$  (Born approximation).

In general, in band structure methods the electron and positron wave functions can be presented as

$$\phi_{\mathbf{k}}^j(r) = \sum_{lm} F_{lm}(k, j, r) Y_{lm}(\hat{r}), \quad (5)$$

where  $Y_{lm}(\hat{r})$  are spherical functions.

While calculating momentum dependent enhancement factors, the most interesting region of momenta  $k$  are momenta close to the Fermi surface. In this region the enhancement factors have the largest values (at least in the case of a homogeneous electron gas) and their variations with momentum are faster. This is due to transitions of electrons from occupied states close to the Fermi surface to free states above it and the contribution to the enhancement from particular non-occupied states is the greatest for  $k' \approx k_F$ . This, in turn, is connected with a small change in positron momentum which leads to a small energy denominator in (2). Thus, the investigation of matrix elements can be limited here to such ones for which the positron momentum  $s$  is small and its orbital quantum numbers are not greater than 2.

The matrix element  $M_{kk's}^{j\alpha\beta}$  is the double integral over  $r_+$  and  $r_-$ . Using the Bloch properties of electron and positron wave functions one can write it for a given  $R_+$  ( $R_+$  and  $R_-$  are lattice vectors connected with appropriate positron (electron) positions) as

$$M = N \sum_{\substack{R_- \\ (\text{near} \\ \text{neighbours})}} M(R_- - R_+), \quad (6)$$

where  $M(R_- - R_+)$  is the double integral over electron and positron coordinates inside the elementary cell. For  $R_- = R_+$  the positron is considered to be located in the same cell as the electron.

In practice the sum in (6) will contain the term  $M(0)$  corresponding to the electron and the positron in the same elementary cell and additional terms for the two particles in neighbouring cells. This is due to the finite range of the e-p interaction which limits the volume of interest in the integration of Eq. (3). We assumed below that the interaction depends only on the distance between given electron and positron.

Now, expanding the e-p potential with respect to spherical harmonics  $Y_{lm}$ , integrating formally over  $r_+$  and making use of some relations between spherical functions, one can present the double integral  $M(0)$  as the expansion with respect to various functions  $G_{lm}$ , where

$$G_{l,m}(s) \equiv G_{lm}(s, i, r_-) = \int dr_+ r_+^2 V_l(r_+, r_-) F_{lm}^{+*}(s, i, r_+) \phi_0(r_+), \quad (7)$$

and come to the following formula:

$$\begin{aligned} M(R_- - R_+) \Big|_{R_- = R_+} &= \int dr_- r_-^2 \sum_{l,m} F_{lm}(k) \left\{ \frac{1}{\sqrt{4\pi}} G_{00}(s) F_{lm}^*(k') \right. \\ &+ \frac{\sqrt{3}}{\sqrt{4\pi}} G_{10}(s) [b_{lm} F_{l+1,m}^*(k') + b_{l-1,m} F_{l-1,m}^*(k')] \\ &- \frac{\sqrt{3}}{\sqrt{8\pi}} G_{1,-1}(s) [-a_{l,-m} F_{l+1,m-1}^*(k') + a_{l-1,m-1} F_{l-1,m-1}^*(k')] \\ &\left. + \frac{\sqrt{3}}{\sqrt{8\pi}} G_{1,1}(s) [a_{l,m} F_{l+1,m+1}^*(k') - a_{l-1,m-1} F_{l-1,m+1}^*(k')] \right\}. \quad (8) \end{aligned}$$

We present here only the first few terms of this expansion. According to previous arguments we shall not take into account terms connected with such positron states for which  $l > 2$ .

We have found that the following interesting selection rules exist in (8): particular positron functions are connected only with the appropriate electron functions and not all combinations of the functions exist. For example, if the positron scatters from one state of orbital quantum number  $s$  to another  $s$  state, one has to take into account electron scattering only from a given  $lm$  state to the same one (of course the momenta  $k$  and  $k'$  may be different). If the positron scatters from  $s$  to  $p$  state, then the selection rules allow for the scattering of the electron only from the state  $lm$  to such ones for which its orbital quantum number changes by unity. For all other combinations of scattered states the corresponding integrals in  $M$  must vanish. For instance, the term with  $F_{lm}(k)G_{1,1}(s)F_{l+1,m+1}^*(k')$  under the integral exists, but the term containing the functions  $F_{lm}(k)G_{1,1}(s)F_{lm}^*(k')$  vanishes.

Let us remark that in the case of scattering of only the electrons on the static potential (e.g. the proton) one could observe only  $k, l, m \rightarrow k', l, m$  transitions, i.e. only the first term in (8) (in which  $G_{00}$  would be just equal to  $V(r)$ ) would remain.

Concerning the number  $m$  of the electron state, the positron changes it only if its number  $m$  is different from zero. Of course, these are the leading terms of the above expansion. The formulae for the remaining ones (e.g. corresponding to the case  $R_+ \neq R_-$ ) are more complicated, but they also contribute less to the matrix element because of the limited range of the e-p interaction.

The calculation of matrix elements seems to be almost impossible task because of the big number of possible combinations of  $l$  and  $m$ . However, after more detailed studies of the properties of band structure wave functions, in particular of the quantities  $F_{lm}(k, n, r)$  it turns out that many of them are equal to zero for some  $l$  and  $m$  because of symmetry. By now this results from numerical calculations, although we expect that it could be proven analytically since it should result from symmetry.

In turn, some of the  $F_{lm}$  functions for different  $m$  are identical as functions of  $r$ . This may simplify the calculations considerably. For example, for  $l = 0, 1, 2$  we have in general 18 real functions (9 complex functions  $F$ ) but practically, for e.g. the  $(-1, -1, 0)$  direction in Cu one must know 2 or 4 (depending on the band) real functions, the rest is only a combination of the last ones. Summarizing, not all possible combinations of  $F_{lm}$  occur in (8) and, moreover, most of those occurring vanish.

As these results are preliminary, we can present only the general rules for the selection of particular electron and positron states when the particles scatter with very low momentum transfer in real metals. We are convinced, however, that just this way of calculating of matrix elements may help to understand which and how realistic electron and positron states actually participate in scattering processes.

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