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Electron–positron correlations in jellium within the self-consistent Kahana approach

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Abstract. The role of the electron–positron enhancement factor $\varepsilon(p)$ in investigations of the electronic structure of metallic materials by positron annihilation is emphasised. A calculation of this function, performed according to a self-consistent extension of the Kahana formalism, is presented. The merits of this approach in comparison with the traditional approach comprise inclusion of the effect of electron–electron correlations and the achievement of full self-consistency between the potential assumed in the Bethe–Goldstone equation and the screening charge distribution around a positron, obtained from its solutions. In this way the low-density divergence of the annihilation rate λ is removed—in this region it approaches the averaged free-positronium value. The annihilation parameters obtained in this work are in reasonable agreement with experimental results.

The momentum-dependent enhancement factor $\varepsilon(p)$ is one of the most important parameters necessary for interpreting positron annihilation data for metals. Once this function is known, the momentum distribution of annihilation photons in real metals can be obtained in the local-density approximation from the formula (Daniuk *et al* 1985, 1987)

$$N(\boldsymbol{p}) = \sum_{k,n} \left| \int \sqrt{\varepsilon[r_s(\boldsymbol{r}), T_{k,n}(\boldsymbol{r})]}\, \psi_{k,n}(\boldsymbol{r})\psi_+(\boldsymbol{r}) \exp(-\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{r})\, \mathrm{d}\boldsymbol{r}^2 \right. \tag{1}$$

where ψ_+ is the wavefunction of the positron in a ground state, $\psi_{k,n}(\boldsymbol{r})$ denotes the wavefunction of the electron with the wavevector $\boldsymbol{k}$ in the nth band, $r_s(\boldsymbol{r})$ characterises the local electron density and $T_{k,n}(\boldsymbol{r})$ is the local kinetic energy.

However, the theoretical calculation of $\varepsilon(p)$ is very difficult, even for such a simple model as an electron gas (Kahana 1963, Maldague 1979, Arponen and Pajanne 1979, Lowy 1982). Of the approaches enabling us to compute these parameters the formalism proposed by Kahana (1963) (and developed by many researchers) is the best known.

The Kahana approach is based on the Bethe–Goldstone equation

$$\chi(\boldsymbol{p},\boldsymbol{k}) = \frac{A\nu(|\boldsymbol{k}-\boldsymbol{p}|)}{k^2 + (\boldsymbol{k}-\boldsymbol{p})^2 - p^2} + \frac{A\nu(|\boldsymbol{k}-\boldsymbol{p}|)}{k^2 + (\boldsymbol{k}-\boldsymbol{p})^2 - p^2} \int_{q>1} \nu(|\boldsymbol{k}-\boldsymbol{q}|)\chi(\boldsymbol{p},\boldsymbol{q})\, \mathrm{d}^3\boldsymbol{q} \tag{2}$$

for the Fourier coefficients of the electron–positron pair wavefunction

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$$\psi_p(\boldsymbol{x}_e, \boldsymbol{x}_p) = \frac{1}{\Omega}\exp(i\boldsymbol{p}\cdot\boldsymbol{x}_e) + \frac{1}{\Omega}\sum_{k>1}\chi(\boldsymbol{p},\boldsymbol{k})\exp(i\boldsymbol{k}\cdot\boldsymbol{x}_e)\exp[i(\boldsymbol{p}-\boldsymbol{k})\cdot\boldsymbol{x}_p]$$

where $\boldsymbol{x}_e$ and $\boldsymbol{x}_p$ indicate the electron and positron coordinates, respectively, $\nu(q)$ is the Fourier transform of the effective electron–positron interaction potential $\nu(|\boldsymbol{x}_e - \boldsymbol{x}_p|)$, $\boldsymbol{p}$ is the initial momentum of the electron, Ω is the volume of the sample, $A = (4\pi^3 k_F a_0)^{-1} \simeq 0.33 r_s/8\pi^2$, where k_F is the Fermi momentum and all momenta are expressed in units of k_F.

It should be pointed out that the Kahana formalism does not include self-consistency between the Coulomb potential assumed in the Bethe–Goldstone equation and the screening cloud distribution obtained from its solutions. On the contrary, because of the strong dependence of the resulting annihilation parameters on the potential used in the Kahana equation (2) (Boroński *et al* 1981, Rubaszek *et al* 1984, Rubaszek and Stachowiak 1984, 1988), definitive and reliable conclusions about the total and partial annihilation rates could be drawn only after achieving full self-consistency in the Kahana approach in the sense of the Hartree–Fock-type (instead of the Poisson) equation

$$q^2[\nu(q) - \nu^{exc}(q)] = -4\pi[1 - \Delta\rho(q)] \tag{3}$$

where $\nu^{exc}(q)$ is the electron–electron exchange and correlation potential and $\Delta\rho(q)$ denotes the electronic screening charge distribution in momentum space.

In this work the Kahana equation (2) is solved self-consistently for $r_s = 2, 4, 6$ and 8 and the resulting annihilation parameters are calculated. The screening charge distribution $\Delta\rho(r)$ was determined from the formula (for details see Rubaszek and Stachowiak (1988)).

$$\Delta\rho(r) = \sum_{k}^{occ}\int d^3\boldsymbol{x}_p\, \psi_k^*(\boldsymbol{x}_p, \boldsymbol{x}_p + \boldsymbol{r})\psi_k(\boldsymbol{x}_p, \boldsymbol{x}_p + \boldsymbol{r}) - \rho_0.$$

In order to avoid the divergence of the potential $\nu(q)$, occurring for momenta close to zero ($q \to 0$) when equation (3) is applied directly and $\Delta\rho(q=0) \neq 1$, the Hartree–Fock equation (3) was replaced in the iterative scheme by (cf also Manninen *et al* (1975))

$$\nu_{n+1}(q) = \{-4\pi[1 - \Delta\rho_n(q)] + \beta^2\nu_n(q) + q^2\nu_n^{exc}(q)\}/(q^2 + \beta^2) \tag{4}$$

where ν_n and ν_n^{exc} are the Coulomb and exchange–correlation potentials, respectively, calculated in the nth iterative step and $\Delta\rho_n(q)$ is the screening charge distribution obtained from the exact solutions of the Kahana equation (2) with the potential ν_n.

The electron–electron correlations were taken into account in a local way by replacing in the exchange–correlation potential of Hedin and Lundqvist (1971) the density of a homogeneous electron gas by the local electron density

$$r_s(r) = \{\tfrac{4}{3}\pi[\rho_0 + \Delta\rho(r)]\}^{-1/3}.$$

It should be stressed here that after applying equation (4) with the constant $\beta^2 > 0$ the potential $\nu_{n+1}(q)$ is well defined for momenta q close to zero because the right-hand side of equation (4) is finite for $q \to 0$ even when the total screening charge, obtained from solving equation (2), is not exactly equal to one electronic charge. The value of β^2 was initially chosen to be equal to $0.33 r_s$ and with increasing convergence of the procedure it decreased. As the first iterative step $\nu_1(q)$ in the procedure (4), the quadratic response theory potential (Rubaszek and Stachowiak 1984) was applied. The calculations were pursued until the condition

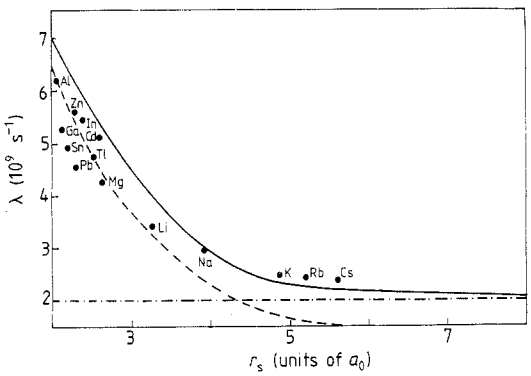

Figure 1. Annihilation rate λ as a function of r_s (———) compared with the results obtained when the electron–electron correlations were neglected (– – –).

$$\max_q |[\nu_{n+1}(q) - \nu_n(q)]/\nu_n(q)| \leq 1\%$$

was satisfied.

The resulting total screening charge around a positron was found to be equal to one electronic charge within an error of about 0.5%. The total annihilation rates λ obtained in this work are shown in figure 1 (full curve) as a function of r_s. The results obtained when the electron–electron correlations were neglected are presented for comparison (broken curve). It can be seen that the agreement between the theoretical and experimental values of λ is very good in the whole region of metallic densities. No low-density divergence (typical of the original Kahana theory) is observed. Inclusion of the electron–electron correlations leads to an increase in the annihilation rates so that it avoids falling below the positronium value $\lambda_{pos} \simeq 2 \times 10^9\ s^{-1}$ (Rubaszek and Stachowiak 1984, Bhattacharyya and Singwi 1972, Lowry and Jackson 1975, Gondzik and Stachowiak 1985).

The relative enhancement factor $\gamma = [\varepsilon(1) - \varepsilon(0)]/\varepsilon(0)$ on the Fermi surface (Rubaszek and Stachowiak 1985) as a function of r_s is presented in figure 2 as a full curve. The biparabolic analogue of γ, $(b + c)/a$ (according to the biparabolic Kahana approximation $\varepsilon(p) \simeq a + bp^2 + cp^4$, the validity of which was discussed by Rubaszek and Stachowiak (1984, 1985)) is shown in figure 2 as a dotted curve. The broken curve labelled (AP) corresponds to the results of Arponen and Pajanne (1979) for $(b + c)/a$ and the broken curve labelled (L) represents the values of γ extracted from the paper by Lowy (1982). The experimental predictions are intermediate between the two parameters: γ and $(b + c))/a$ (cf Rubaszek and Stachowiak 1985).

The comparison of enhancement factors obtained from various theories with the experimental data shows that the present approach agrees better with experiment than other approaches do, at least for low electron densities ($r_s \geq 4$).

With these considerations, we treated real metals as an electron liquid with an appropriate electron density. Calculations using equation (1) have hitherto only been performed to a limited extent (Daniuk *et al* 1985, 1987). It seems that using equation (1) appreciably improves the agreement between theory and experiment (Kontrym-Sznajd *et al* 1988).

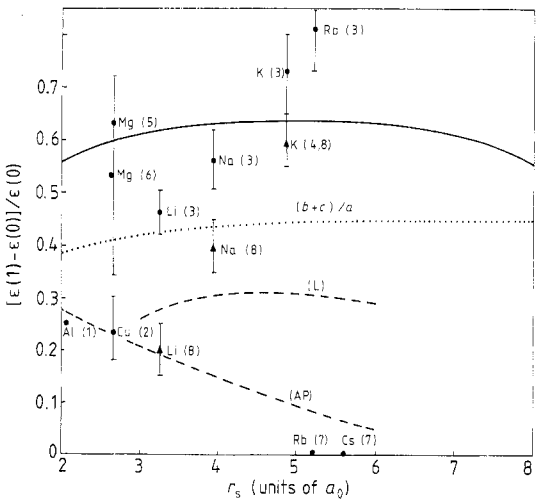

Figure 2. Relative enhancement factors on the Fermi surface (———) compared with their biparabolic analogue $(b + c)/a$ (. . . .); – – – (AP), results of Arponen and Pajanne (1979); – – – (L), results of Lowy (1982). The experimental data are quoted in the paper by Rubaszek and Stachowiak (1988).

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