

high-energy relation between the two cross sections, in which relation K is an energy-independent factor.

$$Q_B(1s) = Q_{BK}(1s) [1 + 5/64(1 + 1/Z)^2 - 5/12(1 + 1/Z)] \\ = 0.535 Q_{BK}(1s), \quad Q_{BK} = KE^{-6}.$$

A final point of interest that emerges from this approximate calculation is the fact that the passive electron interaction V_{p1} , [see Eq. (1a) of I] does not contribute to the high-energy Born cross section. That is, the integration over \mathbf{x}_1 provides a cancellation of one of the proton-nuclear terms, $|\mathbf{x}_2 - \mathbf{x}_3|^{-1}$; however, the residual part of V_{p1} , the exponential term, supplies a high-energy term which replaces the original cancellation. This means that the effective interaction at high energies is

$$2|\mathbf{x}_2 - \mathbf{x}_3|^{-1} - |\mathbf{x}_2|^{-1}.$$

These mathematical details are consistent with the calculations of others.⁵

Note added in proof. This author is currently calculating BK cross sections for electron capture from O(³P) and N(⁴S) by protons. These results, together with the ratios of this paper, will be used to estimate the corresponding Born cross sections. This material will be included in a forthcoming publication.

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Enhancement of Electron Density around Positive Point Charges in Metals and Lifetimes of Positrons

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By means of approximate self-consistent field calculations using a model of a finite metal with ~ 2000 electrons, it is shown that over the range of densities appropriate to metals under normal conditions, the density at the position of a single positive charge varies by a factor of about 2, whereas the variation in the mean electron density ($3/4\pi r_s^3$) is an order of magnitude greater. In a simple Hartree calculation of the type reported here, a bound state occurs when $r_s > 4$ atomic units. Some brief remarks are made on the application of these results to the calculation of the lifetimes of positrons in various metals.

WE report in this note the results of some numerical calculations which we have carried out to estimate quantitatively the enhancement of the electron density around a single positive point charge in a metal. In earlier work we used both a finite metal model for finding electronic wave functions around a vacancy¹ and later we developed a density matrix approach based on low-order perturbation theory² which enabled us to pass to the limit of an infinite metal. Our earlier work¹ indicated that significant results could be obtained using as a model of a metal a finite spherical system containing 1734 particles in 867 doubly filled states and in such a model we have imposed approximate self-consistency in the Hartree sense when a single positive charge is placed at the origin. Mean interparticle spacings measured by r_s values³ of 2, 2.66, 4, 5, and 6 have been considered and usually five or six iterations proved sufficient for achieving satisfactory self-consistency. In

each case we have taken the same number of particles and have obtained different r_s values by altering the size of the spherical system.

The main features of these results are then found to be as follows: First of all, as r_s is increased, we reach a point at which a bound state breaks off from the band. Our finite metal computations indicate that this is occurring when $r_s > 4$. The behavior of the electron density at the origin, denoted by $\rho(0)$, does not show any marked change due to the formation of a bound state, as may be seen from Table I below, which summarizes our results for a range of r_s values covering all metals under normal conditions.

It seemed useful to fit the numerical results given in the table by a simple analytical formula and we did this as follows. Two values of $[\rho(0) - \rho_0]/\rho_0$ were obtained for each value of r_s corresponding to the upper and lower bounds of $\rho(0)$ which differed by a few parts in a thousand. When polynomials with zero constant term were fitted to various groups of points, the quartic terms were found to be very small and random. It was found that a cubic could be constructed which lay within the bounds for each r_s . The formula which gave the best

¹ N. H. March and A. M. Murray, Proc. Roy. Soc. (London) **A256**, 400 (1960).

² N. H. March and A. M. Murray, Proc. Roy. Soc. (London) **A261**, 119 (1961).

³ The mean electron density $\rho_0 = 3/4\pi r_s^3$. We use atomic units (au) throughout.

TABLE I. Summary of results for $\rho(0)$.

r_s (au)	2	2.66	4	5	6
$\rho(0)$	0.396	0.298	0.224	0.201	0.188
ρ_0	0.0298	0.0127	0.00373	0.00191	0.00111
$\rho(0)/\rho_0$	13	23	60	105	169

fit over the whole range considered was

$$[\rho(0) - \rho_0]/\rho_0 = 2.23r_s + 0.766r_s^2 + 0.593r_s^3. \quad (1)$$

On the basis of (1) it is now possible to obtain an estimate of the errors which may be occurring due to our use of a finite metal.⁴ Thus, in our self-consistent perturbation calculations,² we showed that as $r_s \rightarrow 0$,

$$[\rho(0) - \rho_0]/\rho_0 = 2.46r_s, \quad (2)$$

and by comparing the coefficients of the leading terms in (1) and (2) for small r_s , it seems likely that errors of $\sim 10\%$ may be introduced by our finite-metal assumption. This is still much less than the errors in the density at the origin as given by the self-consistent perturbation calculations² applied to the range $2 < r_s < 6$, even when these are extended to include second-order terms.

When we embarked on the present calculations, our aim was to study the variation of positron lifetimes in metals over a wide density range. However, in the meantime, Kahana⁵ has examined this problem in a different, and more sophisticated way, by solving a Bethe-Goldstone equation. For this reason, while we feel that our computations should still be put on record, we restrict ourselves to a very brief discussion of the lifetime problem.

Our principal conclusion which is immediately apparent from Table I is that the variation of lifetimes to be expected through the range of metallic densities is much less than might have been supposed naively from

⁴ The more difficult question as to the range of validity of a Hartree treatment will be referred to a little later.

⁵ S. Kahana, Phys. Rev. **117**, 123 (1960).

the wide variation in the unperturbed density, and this is essentially similar to the finding of Kahana.⁶ From a recent extensive tabulation of experimentally determined lifetimes by Bisi *et al.*,⁷ it may be seen, however, that any approach such as ours, based on the free electron model, can only hope to account for gross features, and doubtless, consideration of the influence of the periodic potential of the unperturbed crystal will eventually prove necessary. Such limitations are further emphasized by the fact that for copper metal, for which $r_s = 2.66$. Hence there is no bound state in our model, and we may evaluate the positron lifetime τ from the result⁸

$$\tau = \frac{\rho_0}{\rho(0)} \left(\frac{r_s^3}{1.2} \right) \times 10^{-10} \text{ sec.} \quad (3)$$

From Table I we immediately obtain a lifetime of 0.6×10^{-10} sec to be compared with the most recent experimental result⁷ of 2.3×10^{-10} sec.

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⁶ Concerning the variation of $\rho(0)$ with r_s , it has been pointed out to us that from (1), as $r_s \rightarrow \infty$, $\rho(0) \rightarrow 0.141$, whereas one might expect physically that in this limit the density $\rho(0)$ is just the hydrogen atom electron density $\pi^{-1} = 0.318$, a value more than twice as large. This reflects the breakdown of a Hartree treatment for low densities, but it also serves to reinforce our main conclusion as to the small variation in the electron density at the position of the point charge for $r_s > 2$. This limiting argument, combined with our results, strongly suggests that $\rho(0)$ passes through a minimum at an intermediate value of r_s , but our present work does not enable us to reach a completely definitive conclusion on this point.

⁷ A. Bisi, G. Faini, E. Gatti, and I. Zappa, Phys. Rev. Letters **5**, 59 (1960).

⁸ See, for example, R. A. Ferrell, Revs. Modern Phys. **28**, 308 (1956).