Polarization Effects Accompanying Positron Annihilation in Metals*

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The experimental data available concerning positron annihilation in metals are shown to be consistent with a positron-electron interaction which is the instantaneous limit of the Hubbard effective potential neglecting exchange. This is shown to reduce to a screened Coulomb potential with an expontential cutoff almost twice as large as the usual plasma cutoff. The data also suggest that the effect of electron-electron interactions upon the momentum distribution is smaller than previous calculations indicate.

CORRELATION and exchange effects in dense electron plasmas result in polarization of the plasma; the resulting correlation corrections have been examined and results which depend on the general character of the effective potential are essentially understood. It is clear that no static effective potential applies, but excellent results are obtained using static potentials since many phenomena are insensitive to the detailed form of the interaction as long as it "cuts-off" at large distances with an appropriate range. Variations in the way the effective potential tends to zero tend to be relatively unimportant in quantities averaged over the full range of the interaction.

The correlation and exchange effects will be important in determining the form of the transformed potential for small momenta and a phenomenon which is determined by this region of the momentum transform would relate to these particular effects. Any phenomenon which involves excitation from the Fermi sea to low-lying levels above it by this potential would be of this nature since the excitation can be expected to drop off strongly at higher energies in the usual manner. In the diffusion of a positron into a metal and its subsequent annihilation, the electron gas is polarized and the electron density at the positron is enhanced, with an associated change in the annihilation rate. That the polarization effect can be thought of as a scattering into states outside the Fermi surface by an effective potential, $V(x'-x)$, follows from the work of Hubbard[1]; the potential $V(x'-x)$ depends on both space and time coordinate differences and is, in general, complex. This effective potential follows from the Coulomb potential $v(x,x')$ between particles at space-time points x and x' by inclusion of the photon self-energy parts, giving an effective photon propagator and potential corresponding to inclusion in the interaction of the polarization effects in the medium.

Kahana[2] has discussed the annihilation rate R in two papers. In the first the Bohm-Pines momentum cutoff is used, i.e., the potential is assumed to be static and its momentum transform set equal to zero for momenta $k<k_c$. A Schrödinger equation results which is solved numerically. In the calculation of Kahana (II) a more suitable static potential is used. Examination of Eqs. (A1) and (A4)[2] shows that the problem is reduced to the previously considered one, except that Hubbard's $V(\mathbf{k},\omega)$ is used in the $\omega=0$ limit; $V(\mathbf{k},\omega)$ is the Fourier transform in both space and time variables of $V(x'-x)$. This reduces the interaction to a static potential and eliminates the imaginary part of V. The results for Al, Li, and Na are within the errors to be expected and the experimental deviations, but a serious criticism of this calculation is the use of the $\omega=0$ limit as a static potential. This is defended on the basis that the results in the high-density limit are essentially independent of this choice. However, since the relaxation time of the electron plasma is small in the high-density limit, the potential will reduce to a static potential in this limit in any case; the justification is not relevant. The static limit (or, more properly, the instantaneous limit) is obtained by replacing the Fourier transform by the infinite frequency limit $\omega\rightarrow\infty$, rather than the zero frequency limit. Deviations from this limit for smaller ranges of ω will produce a nonstatic "retarded" contri-

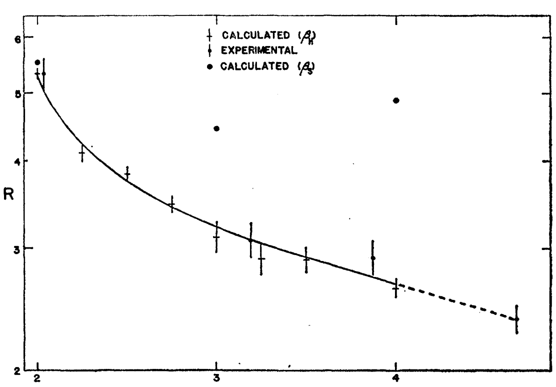

FIG. 1. Calculated variation of annihilation rate with r_s and the experimental data for the alkali metals. Curve is a smooth fit to the calculated points.

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[1] J. Hubbard, Proc. Roy. Soc. (London) **A243**, 336 (1957).
[2] S. Kahana, Phys. Rev. **117**, 123 (1960), Paper I; S. Kahana, *ibid.* **129**, 1622 (1963), Paper II.

bution of duration inversely proportional to the range of this deviation, in the usual manner.

The potential obtained by Hubbard is

$$V(\mathbf{k},\omega)=v(\mathbf{k})/1-V^*(\mathbf{k},\omega),$$
$$V^*(\mathbf{k},\omega)=A(\mathbf{k},\omega)+i\Sigma(\mathbf{k},\omega),$$

in his notation. $v(\mathbf{k})$ is the Fourier transform of the instantaneous Coulomb potential and $V^*(\mathbf{k},\omega)$ is an auxiliary quantity introduced for computational reasons and which Hubbard systematically obtains from a perturbation analysis. He shows $\Sigma(\mathbf{k},\infty)=0$ and

$$A(\mathbf{k},\infty)=\lim_{\omega\to\infty}\frac{\xi}{x^3}\left\{x+\frac{1}{2}\left[1-\frac{1}{4}\left(\frac{y}{x}-x\right)^2\right]\times\ln\left|\frac{y-x(x+2)}{y-x(x-2)}\right|+\frac{1}{2}\left[1-\frac{1}{4}\left(\frac{y}{x}+x\right)^2\right]\times\ln\left|\frac{y+x(x+2)}{y+x(x-2)}\right|\right\}$$

with $x=k/k_F$, $y=\hbar\omega/E_F$ and $\xi=e^2k_F/\pi E_F=0.33r_s$. This limit is

$$A(\mathbf{k},\infty)=-2\xi/x^2=-0.66r_s(k_F/k)^2$$

leading to

$$V(\mathbf{k},\infty)=v(\mathbf{k})/[1+0.66r_s(k_F/k)^2]=v(\mathbf{k})/[1+(k_c/k)^2].$$

This is just the momentum transform of a Coulomb potential with an exponential cutoff. The magnitude of this cutoff is surprising; it is

$$\beta_H=k_c/k_F=0.812r_s^{1/2}.$$

This is much larger than the Bohm-Pines cutoff of $\beta_{BP}=0.353r_s^{1/2}$. Also the work of Sawada, *et al.*[3] indicates that the plasma solutions merge with the pair excitation continuum for momenta of about $0.470r_s^{1/2}$, also much lower than Hubbard's cutoff. β_H is the same as the cutoff obtained by a simple Thomas-Fermi calculation.[4]

We have computed the annihilation rate R using the effective static-potential approximation and assuming that the results are essentially momentum independent, as verified by experiment, so that initial states with $\mathbf{a}=0$ are assumed. We have used $V(\mathbf{k},\infty)$ as the potential transform (we have also checked the results for $\beta_s=0.470r_s^{1/2}$) and find the relative coordinate wave equation

$$u(\mathbf{k})=\frac{1}{k^2(k^2+k_c^2)}+\frac{f}{k^2}\int\frac{u(\mathbf{k}')d^3k'}{|\mathbf{k}-\mathbf{k}'|^2+k_c^2}$$

with $u(\mathbf{k}')=0$, $|\mathbf{k}'|<k_F$. For β_s we have expanded the first term on the right in a binomial series and for β_H we have graphically expanded it to five terms in inverse even powers of k. Writing the integral on the right as

$$I=\frac{f}{k^2}\int\frac{u(\mathbf{k}')d^3k'}{|\mathbf{k}-\mathbf{k}'|^2+k_c^2}=\frac{\pi}{k^3}\int_0^\infty dk'k'u(k')\times\ln\frac{(k+k')^2}{(k-k')^2}-\frac{2\pi}{k^2}u(k)\beta k_F\chi(k_c,k),$$

one can show that $\chi(k_c,k)$ is almost independent of k for fixed k_c and rises with r_s from about $\chi(r_s=2)\approx0.75$ to $\chi(r_s=4)\approx0.85$. The resultant equation was solved by truncation for an r_s range corresponding to physically real substances, $r_s=2.0$ up to $r_s=4.0$, using an IBM-1620 data processor. The rate was obtained by comparing the resulting electron density at the positron to that for singlet positronium.[2]

Recent experimental lifetime data on the alkali metals,[5] for which we would expect good agreement with calculation, are shown in Fig. 1; the flags on our calculated points represent confidence ranges resulting from our approximations. These are large near $r_s=3.01$ due to the accidental cancellation of the leading term in the power-series expansion of $u(k)$ and are large near $r_s=4.0$ due to the fact that the expansion converges very slowly if at all. We carried the calculation to 50 terms and no indication of convergence was obtained for $r_s\gtrsim3.75$. Results were obtained in this range by decreasing $\chi(r_s)$ until convergence was obtained and then performing an extrapolation to realistic values. Lifetimes for $r_s\lesssim2.5$ are quite insensitive to $\chi(r_s)$ and our confidence ranges are correspondingly small. Our results agree with experiment to the accuracy of the calculation for all r_s between $r_s=2.0$ and $r_s=4.0$.

We have also performed the calculation using $\beta_s=0.470r_s^{1/2}$; the results are roughly twice the observed rates. Thus, these results constitute a confirmation of Hubbard's shielding length, neglecting exchange, as a positron-electron cutoff.

Recently, Stewart[6] has obtained sufficiently detailed angular correlation data for the quanta emerging from annihilation in Na to allow the momentum distribution function $\rho(k)$ to be obtained with some precision, assuming the sufficiency of an assumption of spherical symmetry. Our results allow us to calculate the population of states above the Fermi surface $k=k_F$ by polarization of the electronic states in the vicinity of the positron and the reciprocal excitation of the positron.

[3] K. Sawada, K. A. Brueckner, K. Fukuda, and R. Brout, Phys. Rev. **108**, 507 (1957).

[4] See, for example, S. Raimes, *Wave Mechanics of Electrons in Metals* (North-Holland Publishing Company, Amsterdam, 1961), p. 307, or J. M. Ziman, *Electrons and Phonons* (Oxford University Press, 1960), p. 169.

[5] R. E. Bell and M. H. Jorgensen, Can. J. Phys. **38**, 652 (1960); J. L. Rodda and M. G. Stewart, Phys. Rev. **131**, 255 (1963); the latter also contains data on the group III B metals. Additional measurements on metals other than the alkali metals have been made by A. Bisi, G. Faini, E. Gatti, and L. Zappa, Phys. Rev. Letters **5**, 59 (1960); G. Jones and J. B. Warren, Can. J. Phys. **39**, 1517 (1961). A less regular behavior with r_s is observed, as one would expect.

[6] A. T. Stewart, Phys. Rev. **123**, 1587 (1961).

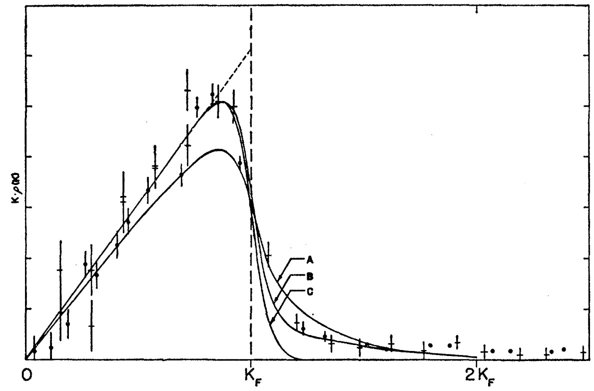

FIG. 2. Curve C is observed using Stewart's resolution curve and the Fermi distribution without corrections. Curve B takes into account the electron-position excitations but ignores electron-electron excitations. If both positron-electron interactions as discussed in this work and electron-electron interaction as computed by Vosko and Daniell are included, curve A results.

The result, normalized to $\frac{4}{3}\pi\rho(k/k_F)=1$ for $k<k_F$ is

$$\begin{aligned}\rho(k/k_F)&=0.239, \quad k<k_F\\ &=5.87\times10^{-3}r_s^2(k_F^4u(k))^2, \quad k>k_F.\end{aligned}$$

This result for $r_s=4.0$ (very close to the $r_s=3.96$ value applying to Na) is shown in Fig. 2 with Stewart's experimental points. The results obtained from an uncorrected Fermi distribution and obtained by taking into account the Vosko and Daniell[7] calculation of the electron-electron excitation in addition to the positron polarization are shown for comparison. These curves are calculated using Stewart's resolution curve to give a predicted experimental $\rho(k)$ curve. It is only that part of the plot near $k=k_F$ which is relevant; the results for k values much larger than k_F will contain uncertain corrections due to annihilation with core electrons as well as the usual background rate, both tending to give an extended tail to the distribution. Such corrections would, of course, make the discrepancy between curve A and the data even larger. In fact, Stewart[6] indicates that an uncorrected Fermi distribution fits the data reasonably well if a considerable background is allowed.

Not only is the effective potential of Hubbard seen to be consistent with experiment, but it is seen that the static limit gives very good agreement. This limit is a Coulomb potential with exponential cutoff. The large value of cutoff predicted is definitely preferred to the cutoff of either Bohm-Pines or Sawada *et al.*

The calculations of the corrections due to electron-electron excitation seem to overestimate this effect. In fact, to the accuracy of the data, almost all annihilations in Na from states above k_F can be attributed to electron-positron excitation; the electron-electron excitations appear to be small in comparison with these.

This raises questions concerning the momentum distribution of an interacting electron gas. At high electron densities the Fermi discontinuity will be more sharply defined than at lower densities. The Vosko and Daniell calculation uses the result of Gell-Mann and Brueckner[8] that the correlation energy of an electron gas follows from electron-hole pair excitations in the high-density limit and does not take into account exchange effects; it is not surprising that the predictions for relatively diffuse electron gases deviate somewhat from the actual situation. Nontheless, the effect of electron-electron corrections seems surprisingly slight.

It is also rather surprising that the cutoff predicted by Hubbard and confirmed by the data of Stewart and the various lifetime data is so large; the result obtained by a simple one-electron Thomas-Fermi calculation is no larger, even though one would expect the operation of the exclusion principle to inhibit the polarization and hence depress the cutoff substantially. While it is true that the Hubbard potential ignores significant exchange terms as an electron-electron potential, these would be small in electron-positron interactions since the positron will not carry an "exchange hole" inhibiting Coulomb correlations. One would surmise that these exchange corrections depress the cutoff for electron-electron interactions so as to correspond to the Sawada *et al.* calculation. It then appears that the Hubbard cutoff (neglecting exchange corrections) provides an excellent positron-electron polarization cutoff but is depressed in electron-electron collisions. A plasma cutoff such as obtained by Sawada *et al.*, allows no distinction between electron-positron and electron-electron interactions; in this sense, the direct approach of Hubbard is to be preferred. The peculiarly small excitation by these electron-electron collisions which Stewart's data allow remains unexplained.

[7] E. Daniell and S. H. Vosko, Phys. Rev. **120**, 2041 (1960).

[8] M. Gell-Mann and K. Brueckner, Phys. Rev. **106**, 364 (1957).