Effective Mass of the Positron in Sodium*

CHANCHAL K. MAJUMDAR
Carnegie Institute of Technology, Pittsburgh, Pennsylvania
(Received 8 April 1966)

The band effective mass of the positron in sodium is computed by the standard method of Wigner, Seitz, and Bardeen. The result is $m^*=1.06m$, where m is the free-particle mass. Combining it with the results of the many-body calculations of the effective mass of a positron interacting with a Fermi sea of electrons, one can conclude that the theoretical value is much smaller than the experimentally observed effective mass.

THE experimental determination of the effective mass of the positron in solids is of some interest since it opens a new way of studying the many-body effects in solids. To our knowledge only one such experiment has been carried out so far by Stewart and Shand[1] in sodium, and a rather high value of the effective mass $m^*=(1.9\pm0.4)m$ has been obtained. A somewhat different analysis of the data leads Brandt *et al.*[2] to conclude that $m^*=1.7m$. Here m is the free-positron mass. In view of the large uncertainty in the experimental value, it is perhaps not unreasonable now to assume that these values are upper bounds for the effective mass; for clearly there are other effects contributing to the smearing of the angular-correlation curve at the Fermi momentum, and selection of the effective-mass contribution is rather difficult.[3]

Preliminary calculations of the band effective mass and the many-body effective mass yielded quite low values, well outside the experimental uncertainty quoted by Stewart and Shand.[4] However, from some calculations à la Landau's Fermi-liquid theory, Ferrell arrived at the conclusion that the many-body effects endow the positron with an effective mass $m^*=2m$.[5] Recently the many-body aspects have been independently studied in great detail by Hamann[6] who believes Ferrell's calculations contain an algebraic error, and corroborates our original conclusion that the many-body effects are too small to account for the observed effective mass. We shall here present our calculations on the band effective mass, which comes out to be $1.06m$, and refer the reader to Ref. 6 for the details of the many-body calculations.

The method followed is the standard technique of Bardeen,[7] which is an extension of the classical Wigner-Seitz[8] method. This was first employed in the positron problem by Berko and Plaskett, for copper and aluminum, and is expected to be entirely adequate for sodium. Our calculation simply confirms the earlier estimate of Dresselhaus[10] that the band effective mass should be close to unity.

I. THE BAND EFFECTIVE MASS

The effective mass of the positron will be changed from the bare value because of two effects: first, the positron moves in a periodic potential of the solid, which we call the "band effective mass," and secondly, it interacts with electrons and phonons in solids, which may together be subsumed under the "many-body effective mass." So far the contribution due to phonons has not been calculated in detail, although this is expected to be small. One can naturally ask which effective mass is relevant to the experimental situation. It is intuitively clear—and a formal justification can be provided—that the many-body effective mass is likely to show up in the experiment. In the metals the positron thermalizes very quickly by interacting with the free conduction electrons, and finally forms a dressed complex with electrons that screen out its long-range Coulomb field. The annihilation radiation arises out of this complex. The operational definition of the effective mass assumes that this positron complex is in thermal equilibrium with the solid and has the same momentum distribution as a classical particle of mass m^* at the temperature of the solid. The band effective mass is of significance only in an indirect way. The above picture looks upon the positron and the electrons in sodium essentially as free particles. While for conduction electrons in sodium such a picture is valid, as known from both theory and experiment, this is not *a priori* justified for the positron without a detailed examination of its band structure. If the positron near the bottom of its ground-state band behaves essentially as a free particle, that is, has an effective mass close to unity, our assumption about its free character is justified. Conversely, if the positron band structure were totally different, for instance, if the band mass came out to be very large or very small compared with unity, one would have to be more cautious in using the electron-positron complex idea. The fact that the band effective mass turns

* Supported in part by the National Science Foundation.
[1] A. T. Stewart and J. B. Shand, Phys. Rev. Letters **16**, 261 (1966).
[2] W. Brandt, L. Eder, and S. Lundqvist, Phys. Rev. **142**, 165 (1966).
[3] C. K. Majumdar, Phys. Rev. **140**, A237 (1965).
[4] C. K. Majumdar, in Proceedings of the International Conference on Positron Annihilation, Wayne State University, July 1965 (to be published). More accurate calculations, part of which is reported in this paper, show that the theoretical values given at that time were actually larger than they should have been.
[5] R. Ferrell (private communication); also reported by A. T. Stewart at the conference mentioned in Ref. 4.
[6] D. R. Hamann, Phys. Rev. **146**, 277 (1966).
[7] J. Bardeen, J. Chem. Phys. **6**, 367 (1938).
[8] E. P. Wigner and F. Seitz, Phys. Rev. **43**, 804 (1933).
[9] S. Berko and J. Plaskett, Phys. Rev. **112**, 1877 (1958).
[10] G. Dresselhaus, J. Phys. Chem. Solids **1**, 14 (1956).

out to be close to unity dispels any doubt on this point; the effect of the periodic potential is indeed small.

In calculating the band mass of the positron, we ignore the electron-positron correlation altogether. In other words, the electronic charge distribution remains identical to that in the absence of the positron. The solid as a whole is electrically neutral, and the potential experienced by the positron in each unit cell is repulsive. The repulsion is of nuclear origin and is therefore concentrated in a very small region in the unit cell. The electrons screen out the repulsion almost completely over most of its volume. The potential felt by the positron may thus be regarded as weak and the positron wave function differs from the plane wave only very little.

Since the methods of calculation are quite well known and the details involve a mass of numbers, only an outline will be given. We attempt to compute the wave function of the positron correct to first order in the wave vector $\mathbf{k}$, which gives the energy correct to $O(\mathbf{k}^2)$, the linear term vanishing by symmetry. The coefficient of the $\mathbf{k}^2$ term is related to the effective mass. The wave function for the positron for the state of wave vector $\mathbf{k}$ can be written as

$$\psi_{\mathbf{k}}(\mathbf{r})=e^{i\mathbf{k}\cdot\mathbf{r}}[u_0(r)+i\mathbf{k}\cdot\mathbf{r}v(r)]. \tag{1.1}$$

Write now

$$u_0(r)=R/r, \tag{1.2}$$

and

$$v(r)=P/r^2-R/r. \tag{1.3}$$

Substituting (1.1) in the Schrödinger equation and using Bardeen's argument,[7] one can show that R satisfies an s-wave equation

$$d^2R/dr^2+2m/\hbar^2[E_0-V(r)]R=0, \tag{1.4}$$

with the boundary condition

$$(dR/dr)_{r_s}=R(r_s)/r_s, \tag{1.5}$$

corresponding to the usual condition

$$(du_0(r)/dr)_{r_s}=0 \tag{1.5'}$$

on the Wigner-Seitz sphere of radius r_s. This determines the ground-state energy E_0. Now P in Eq. (1.3) satisfies a p-wave Schrödinger equation with the same energy E_0:

$$\frac{d^2P}{dr^2}-\frac{2}{r^2}P+\frac{2m}{\hbar^2}[E_0-V(r)]P=0. \tag{1.6}$$

There is one solution of this equation finite at the origin; its scale factor is fixed by the boundary condition that

$$v(r_s)=0, \tag{1.7}$$

or

$$P(r_s)=r_sR(r_s). \tag{1.7'}$$

One can now integrate (1.4) and (1.6), in general numerically, when $V(r)$ is known. The total energy correct to order $\mathbf{k}^2$ is

$$E=E_0+(\hbar^2k^2/2m)\alpha, \tag{1.8}$$

where α is given by[11]

$$\alpha=\gamma\left[\frac{r}{P}\frac{dP}{dr}-1\right]_{r_s}, \tag{1.9}$$

and

$$\gamma=\tfrac{4}{3}\pi r_s^3[u_0(r_s)]^2. \tag{1.10}$$

γ is the ratio of the square of the s-wave function at the Wigner-Seitz sphere to its mean value in the sphere. The reciprocal of α gives the effective mass m^*.

For the potential we have used

$$V(r)=\frac{Ze^2}{r}-\sum_{i=1}^{z}\int\frac{e^2}{|\mathbf{r}-\mathbf{r}'|}|\varphi_i(\mathbf{r}')|^2d\mathbf{r}'. \tag{1.11}$$

ϕ_i's are properly normalized electron wave functions. Z is of course 11 for sodium. The ten inner-core electron wave functions were taken to be the atomic wave functions as given by Kennard and Ramberg,[12] and the conduction-electron wave function is that given by Callaway.[13] The problem of computing (1.11) is then reduced essentially to ordinary electrostatics with some straightforward angular-momentum algebra. The calculation of the resulting radial integrals is performed numerically. Consistent with our approximation scheme, $V(r)$ is a function of the radial distance alone.

The differential equations (1.4) and (1.6) were integrated numerically by standard methods.[14] Figure 1 represents these wave functions. The solution u_0 at energy $E_0=0.080$ a.u. satisfies the boundary condition (1.5') at the Wigner-Seitz sphere radius $r_s=3.94$ a.u. appropriate for sodium. Correspondingly the p-wave function at $E_0=0.080$ a.u. is also shown with a reduced scale. To give an idea of the accuracy of the calculated value of m^* we have also plotted two other wave functions obtained as solutions of (1.2) at neighboring energies of 0.07 and 0.09 a.u., and the corresponding p-wave solutions for Eq. (1.6). These two of course do not satisfy the boundary condition (1.5'). Here we collect the three values of the effective mass:

Energy (a.u.)	m^*/m
0.070	0.95
0.080	*1.06*
0.090	1.21.

The correct band effective mass is therefore 1.06 times the free mass. The variation with energy is sufficiently small, so that any possible error in the energy determination by (1.5') does not change the value appreciably.

---

[11] For a derivation of this equation from variational methods see W. Kohn, Phys. Rev. **87**, 472 (1952).

[12] E. Kennard and E. Ramberg, Phys. Rev. **46**, 1034 (1934).

[13] J. Callaway, Phys. Rev. **113**, 1255 (1961).

[14] D. R. Hartree, *The Calculation of Atomic Structures* (John Wiley & Sons, Inc., New York, 1957), Chap. 4.

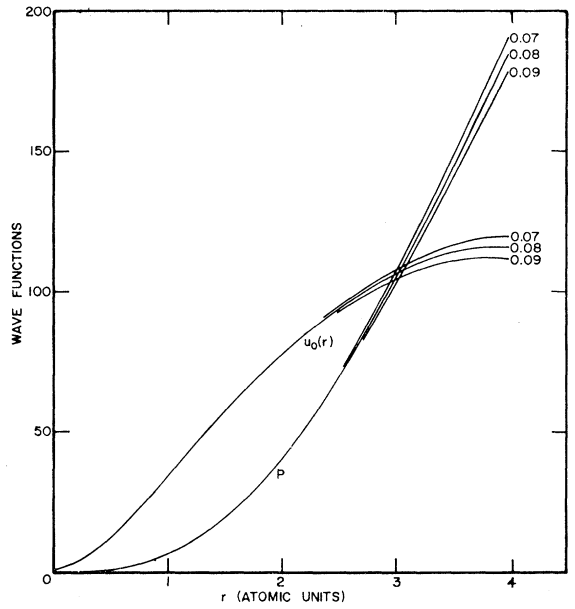

FIG. 1. The wave functions $u_0(r)=R/r$ and P for various energies (in atomic units) as indicated. The scale for the P function is reduced ten times for convenience in plotting. The correct energy is 0.080 a.u.

The over-all reliability of the result depends ultimately on the potential computed from (1.11) and thus on the electronic wave functions. As mentioned earlier, the above calculation takes no account of the distortion of the electronic charge distribution due to the Coulomb force of the positron. This is particularly important for the conduction-electron wave function, since the free electrons will respond rather easily to the positronic attraction and will tend to screen it out effectively. The core electronic wave functions will also be distorted, but not as much as those of the conduction electrons. If one neglects the distortion of the core electronic wave functions, the problem of accounting for the redistribution of the conduction-electron charges belongs legitimately to the calculation of the many-body effective mass. Thus we do not consider it any further.

II. DISCUSSIONS

We have just seen that band effective mass of the positron in sodium is $m^*=1.06m$. The many-body effective mass turns out to be less than $1.18m$, as described in Ref. 6. We can conclude that the present experimental result cannot be explained by these calculations. The phonon part of the many-body effective mass is now under investigation, but is not expected to be large. Before we attempt even more sophisticated calculations, invoking perhaps strong-coupling theories, it would be better to know the experimental value with more certainty. We hope the accuracy of the experimental determination will improve, and more experiments will be done on sodium as well as other suitable materials.

Note added in proof. S. M. Kim of the University of North Carolina has now repeated and confirmed the experimental result. His calculation of the band effective mass is also in essential agreement with the result reported here [to be published in Proc. Phys. Soc. (London)].

ACKNOWLEDGMENTS

It is a pleasure to thank Dr. E. Woll, Dr. J. S. Langer, and Professor S. DeBenedetti for their interest and encouragement. The financial support of the National Science Foundation is gratefully acknowledged.