Positronium Formation in Metals

H. KANAZAWA
College of General Education, University of Tokyo, Tokyo, Japan
AND
Y. H. OHTSUKI AND S. YANAGAWA
Department of Applied Physics, Faculty of Engineering, University of Tokyo, Tokyo, Japan
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A bound-state problem is solved for an extended Bethe-Goldstone equation which includes the short-range positron-electron interaction. It is concluded by numerical calculation that positronium formation is not possible in the usual range of the density parameter r_s.

1. INTRODUCTION

EXPERIMENTS on 2γ annihilation of the positron in crystals are very useful for determining the momentum distribution and the Fermi sphere of the conduction electrons. The thermalization time of the incident positron is much shorter than the lifetime of the 2γ annihilation, and the 2γ angular correlation reflects the momentum distribution of the conduction electrons or the core electrons before the 2γ annihilation.[1] Experimentally, Stewart[2] did the 2γ annihilation for Na crystals, and found that the momentum distribution of conduction electrons is very near that of free electrons. However, the results of Stewart do not agree with the theoretical calculation of Daniel and Vosko.[3] Daniel and Vosko calculated the momentum distribution of electrons in the random-phase approximation, and found that it differs appreciably from that of free electrons because of the Coulomb interaction between electrons. The experimental results of Stewart[2] might be interpreted as follows: The electrons are accompanied by screening clouds and the electron gas is regarded as an assembly of quasiparticles, the momentum distribution of which is calculated by Daniel and Vosko; but when an electron comes very close to the positron, which is also accompanied by a screening cloud, the two clouds cancel each other and the electron annihilates with the positron as a bare electron; thus the 2γ angular correlation reflects the momentum distribution of bare electrons. But the 2γ angular correlation does not correctly reflect the momentum distribution of the conduction electrons in crystals. Thus it is an important problem to investigate the possibility of positronium formation in metals.

Experimentally, it is reported by many authors[4,5] that positronium formation is not possible in various metals. In this paper, starting with the Bethe-Goldstone equation, we discuss theoretically whether or not the formation of positronium is possible in various metals taking into account the Pauli principle and screening effects.

[1] R. A. Ferrell, Rev. Mod. Phys. **28**, 308 (1956).
[2] A. T. Stewart, Phys. Rev. **123**, 1587 (1961).
[3] E. Daniel and S. H. Vosko, Phys. Rev. **120**, 2041 (1960).
[4] R. E. Bell and M. H. Jørgensen, Can. J. Phys. **38**, 652 (1960).
[5] G. Jones and J. B. Warren, Can. J. Phys. **39**, 1517 (1961).

2. BOUND-STATE SOLUTIONS

The Bethe-Goldstone equation for bound states is as follows, taking into account the Pauli principle and screening effects:

$$(\mathbf{k}^2+\mathbf{k}_0^2)\chi(k)=g\sum_{\substack{|\mathbf{k}'|>k_F\\ |\mathbf{k}-\mathbf{k}'|>k_c}}\frac{1}{|\mathbf{k}-\mathbf{k}'|^2}\chi(k') \quad (k>k_F), \tag{1}$$

where $g=4\pi me^2/\hbar^2$, $k_0^2=-mW/\hbar^2$. W is the energy which will be negative if a bound-state solution exists. $\chi(k)$ is a Fourier component of a wave function of the electron-positron pair. k_F and k_c are the Fermi wave number and the screening wave number, respectively, which are related to the density parameter r_s by

$$k_F=1.917/a_0r_s, \tag{2}$$

and

$$k_c=0.470k_Fr_s^{1/2}, \tag{3}$$

where a_0 is the Bohr radius, and $r_s=(3n/4\pi)^{1/3}/a_0$, n being the mean density of conduction electrons.

The right-hand side of Eq. (1) is divided into two integrals, which include the effects of the Pauli principle and the effect of the screening. We have

$$(\mathbf{k}^2+\mathbf{k}_0^2+2\pi xgk_c)\chi(k)=\frac{2\pi g}{k}\int_{k_F}^{\infty}k'dk'\ln\left|\frac{k+k'}{k-k'}\right|\chi(k'), \tag{4}$$

where x is a parameter which indicates the magnitude of the screening effects.[6] We adopt the most reasonable value x with respect to the experimental value of the positron annihilation rates.

Now, since $\chi(k)$ is defined for $k>k_F$, we may expand the wave function $\chi(k)$ as a power series in (k_F/k). It is easy to see that the wave function $\chi(k)$ is an even function of k, and the power-series expansion has the following form:

$$\chi(k)=\sum_{n=0}^{\infty}C_n(k_F/k)^{2n}. \tag{5}$$

[6] S. Kahana, Phys. Rev. **117**, 123 (1960); A. Held and S. Kahana, Can. J. Phys. **42**, 1908 (1964).

If we substitute Eq. (5) into Eq. (4), it is easy to show that $C_0=0$, $C_1=0$. Thus Eq. (4) admits a solution

$$\chi(k)=\frac{1}{k^4}\sum_{n=0}^{\infty}C_n\left(\frac{k_F}{k}\right)^{2n}, \tag{6}$$

with the coefficients in (6) satisfying Eq. (4),

$$C_0=\tau\sum_{n=0}^{\infty}\frac{1}{2n+1}C_n$$

$$C_{r-1}+\lambda C_{r-2}=\frac{\tau}{2r-1}\sum_{n=0}^{\infty}\frac{1}{2n-2r+3}C_n \quad (\text{for } r\geq 2), \tag{7}$$

where

$$\tau=\frac{2}{\pi}\frac{1}{a_0k_F}, \quad \lambda=\frac{k_0^2+2\pi xgk_c}{k_F^2}. \tag{8}$$

Inserting the relation $k_0^2=-mW/\hbar^2$ into Eq. (8), we have

$$W=-\frac{\hbar^2k_F^2}{m}\lambda+\frac{2\pi\hbar^2}{m}xgk_c, \tag{9}$$

or

$$W=27.09\left\{-3.675\lambda\frac{1}{r_s^2}+0.901\frac{1}{\pi\sqrt{r_s}}\right\}\text{ eV}. \tag{10}$$

(Kahana's screening parameter x is assumed to be 1.)

If we can find a positive value λ which makes the energy W negative, we shall have a bound-state solution (a positronium state) for the Bethe-Goldstone equation. From Eq. (9) we must seek a positive value λ which exceeds the value λ_0;

$$\lambda_0=(0.901/3.675\pi)r_s\sqrt{r_s}\sim 0.078r_s\sqrt{r_s},$$

where λ_0 is the value of λ that makes W zero.

3. NUMERICAL CALCULATIONS

We solved a truncated set of Eqs. (7) for $C_n(n=0, 1, \cdots, 9)$ using an electronic computer. We have carried our computations for the different values of the parameter τ. The values $\tau=0.6667$, 1.2500 correspond roughly to aluminum and sodium, respectively. Only positive eigenvalues for different values of τ are shown in Table I. The critical values λ_0 for positronium formation are also shown in the table. It is shown in Table I that there is no positive eigenvalue which exceeds the value λ_0; there is no positronium formation for any value of r_s considered here. If we do not take into account the screening effects, positronium formation occurs at the value $r_s=4.521$. The results show us that the screening effects prevent positronium formation.

TABLE I. Variation of the eigenvalue λ and the critical value λ_0 with valence-electron density.

τ	r_s	β	λ_0	λ
0.667	2.010			
1.000	3.014			
1.250	3.768	0.912	0.570	
1.500	4.521	0.999	0.750	0.41
1.750	5.275	1.080	0.945	0.63
1.825	5.501	1.102	1.006	0.64
2.000	6.028	1.154	1.154	0.64
2.100	6.329	1.183	1.242	0.63
2.250	6.782	1.224	1.377	0.60
2.500	7.535	1.290	1.613	0.60

4. DISCUSSION

A. The Truncated Equations

We computed the truncated set of Eqs. (7) for ten values of $n(n=0, 1, \cdots, 9)$. To estimate the errors of the results we chose three typical values of r_s:

5.275, 6.028, 6.782,

and solved the truncated set at the values of $n=11$, 13, and 15. Thus we calculated numerically the 12×12, 14×14, and 16×16 determinants for the different values of r_s. The computed eigenvalues are shown in Table II. From the table it is roughly concluded that the addition of five more rows and columns only gives a small correction to the eigenvalue when r_s is small. On the other hand, the change of the critical values of λ_0 due to screening effects is very large compared with the change of the critical value due to the dimension n. Thus it is concluded that the truncation of Eq. (7) at $n=9$ does not cause a serious error in the conclusion of the previous sections. However, the results give an incorrect conclusion when the values r_s are large. To make our discussion more accurate, we computed the determinant with five more dimensions (20×20) when $\tau=2.000$ ($r_s=6.028$). Computed results are shown in Table II. Thus these results support our conclusion of Sec. 3.

TABLE II. Computed eigenvalues for determinants of different dimensions and electron densities.

	$\tau=1.750$ $r_s=5.275$	$\tau=2.000$ $r_s=6.028$	$\tau=2.250$ $r_s=6.782$
$m=11$	0.67	0.70	0.60
$m=13$	0.71	0.74	0.65
$m=15$		0.77	0.70
$m=17$		0.80	
$m=19$		0.82	
$m=20$		0.83	

B. x and β

In the present work, we assumed Kahana's parameter x to be 1, and the screening parameter $\beta=k_c/k_F$ to be $0.470r_s^{1/2}$. It was shown by Kahana in his treatment of positron annihilation rates in metals that the rates agree well with the experimental values, assuming x to be 1. Then in our case also it is reasonable to assume x to be 1.

The value $\beta=0.470r_s^{1/2}$ is calculated assuming the conduction electrons of the metal to be an electron gas and assuming the possibility of a high-density expansion ($r_s\leq 1$). In real metals r_s is larger than 1, and the high-density expansion should not be correct. However, it is shown that the theoretical value $\beta=0.470r_s^{1/2}$ agrees with the experimental values for various metals, for example, aluminum ($r_s=2.010$) and sodium ($r_s=3.768$). Thus it is concluded that the results gained in this paper should be correct in the range of small r_s. It is desirable to use the experimental data of k_c in the range of large values of r_s. Unfortunately, we have no experimental data on k_c for large values of r_s. But this fact does not prevent us from concluding that positronium formation does not occur in real metals.

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An Additional Equation in the Phenomenology of Superconductivity: Resistive Effects

P. W. ANDERSON AND N. R. WERTHAMER
Bell Telephone Laboratories, Murray Hill, New Jersey

AND

J. M. LUTTINGER
Columbia University, New York, New York

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We give a phenomenological derivation and a discussion of the "extra Ginzburg-Landau equation" which connects the charge, electrical potential, and time dependence of the order parameter in a superconductor.

RECENTLY Gor'kov[1] pointed out that in his version of the BCS theory of superconductivity the "anomalous" Green's function, $F\sim\langle\psi\psi\rangle$, and thus the energy-gap function Δ and the Ginzburg-Landau order parameter Ψ, vary as $e^{-2i\mu t/\hbar}$, where μ is the Fermi energy. Josephson[2] first noted that this time dependence has observable effects. In particular, it leads to the ac Josephson current in two-superconductor tunnel junctions.

Because of this time dependence, the Fermi level plays a role in the phenomenology of superconductivity different from that in normal metals: it is not only a macroscopic variable determined by local thermodynamic equilibrium, but a microscopic variable determining the local state, which is closely coupled by the long-range order throughout the superconducting circuit.

Corresponding to this duality, we may introduce the chemical potential into the theory in two ways. In both let us first consider an isolated uniform bit of superconductor in equilibrium, later assuming in the standard fashion of nonequilibrium thermodynamics that a steady-state system is made up of many such bits together with the heat and particle flows necessary to maintain quasiequilibrium.

The Hamiltonian of our bit of superconductor is taken as

$$\mathcal{H}=\mathcal{K}+\mathcal{U}_p+\mathcal{H}_{\rm int}+eVN, \tag{1}$$

where $\mathcal{K}$ is the kinetic energy, $\mathcal{U}_p$ is the lattice periodic potential, $\mathcal{H}_{\rm int}$ is the short-range interaction responsible for superconductivity, V is the mean electrostatic potential including any long-range effect due to a net space charge in the sample, and N is the total electron number. The energy necessary to add a single electron of momentum k in a normal metal with Hamiltonian (1) we define as ϵ_k+eV.

In the standard version of superconductivity theory we add and subtract a term μN, obtaining

$$\mathcal{H}\equiv\mathcal{H}'+\mu N. \tag{2}$$

Then the quasiparticle energies and the total many-particle state are calculated for the Hamiltonian $\mathcal{H}'$. The quasiparticle energy is

$$E_k=[(\epsilon_k+eV-\mu)^2+\Delta^2]^{1/2},$$

and has a minimum at the "Fermi surface" where $\epsilon_k+eV=\mu$. The Hamiltonian $\mathcal{H}'$ leads to no time dependence of F and Δ. The number of particles N is not fixed, but the mean value may be obtained in the usual fashion,

$$G(\mu,T)=-kT\,\ln\mathrm{Tr}\,\exp(-\beta\mathcal{H}'),$$
$$\langle N\rangle=-\partial G/\partial\mu. \tag{3}$$

[1] L. P. Gor'kov, Zh. Eksperim. i Teor. Fiz. **34**, 735 (1958) [English transl.: Soviet Phys—JETP **7**, 505 (1958)].
[2] B. D. Josephson, Phys. Letters **1**, 251 (1962).