Localized positron state in a simple metal

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An energetically favored state of a positron in a metal is a new state: a neutral formation of finite dimension. This fact is consistent with experimental data on the positron lifetime and on the angular distribution of annihilation γ rays.

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According to the general understanding, a fast positron is thermalized in a metal in a time (10^{-11} s) much shorter than its lifetime in the metal ($\tau \sim 10^{-10}$ s). The annihilation occurs in a state in which the translational kinetic energy of the positron is zero. The present understanding is based on the assumption that the positron is in an unlocalized state.[1–3] In the homogeneous model of a metal (the "jellium" model) an unlocalized positron has a wave function $\psi^+(r) = 1/\sqrt{V} = \text{const}$. When the crystal structure is taken into account, the positron is described by a function of the Bloch type corresponding to the minimum energy of the band.

An unlocalized state, however, does not satisfy the principle of a minimum energy of the positron-metal system. It is energetically more favorable for the positron to form a localized state screened by an electron cloud of unit charge. The formation of a neutral quasiparticle (pseudopositronium, PPs) with a characteristic dimension R results from a competition between the advantage in terms of the Coulomb energy of the interaction of the positron with its cloud ($-1/R$) and the disadvantage due to the increase in the kinetic energy of a positron localized in a well ($1/R^2$). The dimension of pseudopositronium is determined by the density parameter of the electron fluid, $R \sim r_s \sim 1/p_F$. Pseudopositronium begins to form even before thermalization at positron velocities on the order of the electron velocities. The condition for the formation of a quasiparticle is clearly satisfied during the positron lifetime: $\tau(p_F/m) \gg r_s$. In an unlocalized state, a positron does not perturb the electron density (ρ_0), but to satisfy the

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neutrality condition we must assume that the appearance of the positron in the volume is accompanied by the simultaneous appearance of an electron that comes from the surface of the metal and is in a state with the Fermi energy ϵ_F.

The localized state of the positron differs from known self-localization states (e.g., bubbles in He and polarons[4]), which necessarily involve a system of atoms and its deformation. The charge of the self-localization state is not screened, and the mass can reach several times the atomic mass. Neutral pseudopositronium forms as a result of a deformation of the electron fluid; the mass of pseudopositronium does not exceed twice the electron mass.

The energy of pseudopositronium can be calculated in the jellium model. The electron states are found through a self-consistent solution of the nonlinear Hartree-Fock equations with a fixed positron charge density distribution $\rho_+ = |\psi_\mu^+|^2$. The positron wave function is specified by means of variational parameters $\{\mu\}$, whose values are determined from the requirement that the total energy of the system be at a minimum. The difference between the energies of the system with the positron in a localized state ($\tilde{E}_\mu$) and in an unlocalized state ($E_0 + \epsilon_F$) is, in the Hartree-Fock approximation,

$$\omega_\mu = [(\hat{T}\tilde{\rho}) - (\hat{T}\rho_0) - \epsilon_F] + \frac{1}{2}(\delta\rho|Q|\delta\rho) - (\delta\rho|Q|\rho_+) + (\hat{T}\rho_+), \tag{1}$$

where Q is the Poisson integral, $(\hat{T}\rho_+)$ is the kinetic energy of the positron, and the charge of the electron cloud is $\delta\rho = \tilde{\rho} - \rho_0$ ($\int\rho_+ d^3r = \int\delta\rho d^3r = 1$). The simplest form of the normalized function ψ_μ^+ satisfying the conditions for a 1s-wave function in the case of a nonsingular potential is specified by a single variational parameter:

$$\psi_\mu^+(r) = \left(\frac{2\mu^3}{\pi^4}\right)^{1/2} \frac{1}{\mathrm{ch}\mu r}; \quad (\hat{T}\rho_+) = \frac{\mu^2}{16}\left(1 + \frac{8}{\pi^2}\right). \tag{2}$$

The values of μ_0 and ω_0 corresponding to the minimum energy are listed in Table I ($e = m = \hbar = 1$). The exchange interaction of the electrons changes the results slightly. Figure 1 shows a representative distribution of the positron charge density ρ_+ and the charge density of the electron cloud, $\delta\rho$. The results calculated by the Thomas-Fermi method agree within 30% with the results calculated by the Hartree-Fock method. The formation of a localized state is favored over the entire metallic density range.

How does the lattice affect the pseudopositronium? Numerical calculations show that the interaction of pseudopositronium with the neutral charge of a primitive cell of

TABLE I.

r_s	μ_0^{HF}	ω_0^{HF}	ω_0^{TF}	η
2.07 (Al)	0.65	−0.046	−0.050	1.1
3.93 (Na)	0.62	−0.044	−0.047	1.2
4.86 (K)	0.58	−0.043	−0.046	1.3

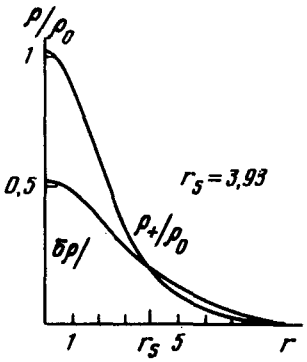

FIG. 1.

a real simple metal, $\Delta\omega_{\mu I} = (\rho_+ - \delta\rho | Q | \Sigma\delta(r - r_i) - \rho_0)$, is negative and small (-10^{-3}). The corresponding quantity for an unlocalized positron state is zero. An estimate of $\Delta\omega_{\mu I}$ from the Wigner-Seitz model also yields a negative value (-0.05); i.e., the lattice promotes the formation of a localized state. Minimizing the expression for the energy $\omega_\mu + \Delta\omega_{\mu I}$, we find the new value $(\mu_{0I} - \mu_0)/\mu_0 \approx -0.1$ for the equilibrium parameter; this value corresponds to a slight expansion of the pseudopositronium in the lattice.

The effective increase in the electron density near the positron causes the rate of annihilation of the localized state ($\tilde{\lambda}$) to be higher than that for the annihilation of an unlocalized state (λ_0):

$$\eta = \frac{\tilde{\lambda}}{\lambda_0} = 1 + \frac{1}{\rho_0} \int d^3 r \delta\rho(r) \rho_+(r). \tag{3}$$

The localization factor η (Table I) augments the known amplification factor[2,3] ϵ which stems from the strong correlation of the annihilating positron and electron at small relative velocities v ($e^2/\hbar v \sim 1$). The localization factor essentially eliminates the discrepancy between theory and experiment regarding the positron lifetime in simple (alkali) metals. In the model of an unlocalized state the discrepancy is attributed to the annihilation of the positron with the valence electrons of ions without regular quantitative calculations.[2]

The formation of a localized state is consistent with data on the angular distribution of the annihilation γ rays. This angular distribution is related to the quantity[1-3]

$$N(k_z) \sim \int dk_x dk_y \Gamma(\mathbf{k})$$
$$\Gamma(\mathbf{k}) \sim \int_0^{\epsilon_F} d\epsilon g(\epsilon) \left| \int d^3 r \exp(i\mathbf{kr}) \psi^+(\mathbf{r}) \varphi_\epsilon(\mathbf{r}) \right|^2, \tag{4}$$

where $g(\epsilon)$ is the electron state density. The localized and unlocalized states of the positron lead to different types of behavior for $\tilde{\Gamma}$, Γ_0 and $\tilde{N}$, N_0 (Fig. 2). Experimentally, the $N(k_z)$ dependence is observed to be smooth, and this is furthermore what we would expect on the basis of a localized state. The model of an unlocalized state (with annihilation by lattice electrons) predicts a jump at $k_z = p_F$.

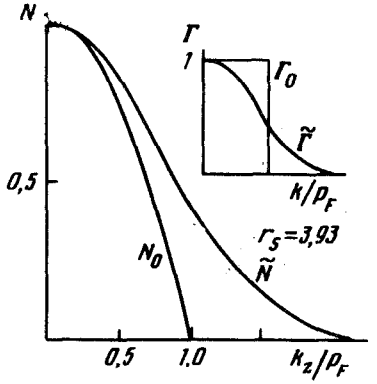

FIG. 2.

These numerical calculations are semiquantitative. Retardation and nonlocality effects may cause the eigenenergy part of the exact formulation of the problem in the theory of finite Fermi systems[5] to differ from the self-consistent Hartree-Fock field and may change the binding energy and the size of the pseudopositronium. The structure features of the pseudopositronium and the details of its interaction with the lattice should be manifested in the diffusion of positrons in a metal with capture by vacancies and also in the emergence of the positrons at the surface.

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