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Positronium in a cavity in a high-T_c superconductor

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Contents

Abstract. The behavior of positronium localized in a microvoid in a high-temperature superconductor (HTSC) environment is examined. The interaction of such a positronium with conduction electrons is treated as arising from the Ps $\leftrightarrow e^+ + e^-$ process, which is mathematically described here in terms of the well-known Anderson model for a magnetic impurity in a normal metal. In this model, the interaction underlying this process is due to the positronium state hybridization with the states of conduction electrons and the state of the positronium remaining within the void. Similarly to the case of a magnetic impurity, the density of states of an interacting positronium exhibits a 'Kondo resonance' if the Fermi liquid surrounding the void is in the normal state. Based on experimental data on the lifetime τ_2 of void-trapped positrons, it is concluded that the hybridization interaction is much stronger than the intra-atomic relativistic electron–positron interaction in the Ps atom. The model used to describe the interacting Ps atom provides a relation between the experimental values of $\tau_2(T)$ and the properties of the electronic structure of the metal. Experimental results for ceramic HTSC samples of $(Bi,Pb)_2Sr_2Ca_2Cu_3O_7$ and (Bi,Pb)-2223 are interpreted, which show a sharp decrease in $\tau_2(T)$ at $T = T_c$, where T_c is the superconducting transition temperature. Using the adopted model, some conclusions are drawn as to how the properties of the pseudogap correlate with the experimental $\tau_2(T)$ dependence observed in (Bi,Pb)-2223 for $T > T_c$.

1. Introduction

Among the many new phenomena that emerged from solid state applications of the positron annihilation method [1 – 7], we here consider one that results from the formation of a bound positron–electron state in a microcavity in a ceramic high-temperature superconductor (HTSC) [8]. Importantly, the properties of such a bound state are not identical to those of common positronium in the vacuum but depend on the interaction of positronium with the surroundings of the cavity and are therefore a convenient probe for the electronic structure of the superconductor in general and, in particular, for the nature of the pseudogap that forms at $T > T_c$, where T_c is the superconducting transition temperature.

With the relativistic nature of the electron–positron interaction in an atom neglected, the quantum mechanics of a positronium atom is very much that of a hydrogen atom. The important difference, however, is that in the Schrödinger equation, the reduced mass of the hydrogen atom $mM/(m+M)$ (where M and m are the proton and electron masses) is replaced with $m/2$, resulting in the ground state binding energy of the Ps atom, 6.8 eV, being half that for H. The relativistic interaction within an atom gives rise to a singlet state I^1S_0 (parapositronium) and a triplet state I^3S_1 (orthopositronium). The ground state of positronium is the I^1S_0 state. The energy difference between the I^3S_1 and I^1S_0 states is 8.4×10^{-4} eV.

The properties of positronium in the vacuum are well described in the framework of quantum electrodynamics. In particular, the interaction of a positronium atom with an electromagnetic field makes positronium unstable. In accordance with the laws of quantum electrodynamics, para- and orthopositroniums respectively transform (annihilate) into two and three γ quanta, with the respective lifetimes 1.25×10^{-10} s and 1420×10^{-10} s.

The formation of Ps in a solid depends on and is correlated with the internal properties of the solid. Under certain conditions, positronium is formed with properties determined by the relativistic intra-atomic interaction, but its lifetime is smaller (especially for orthopositronium). The reason is the so-called 'pick-off' annihilation, an effect in which the component positron of Ps annihilates with an electron from the surrounding medium. The formation of Ps with its relativistic properties preserved requires that there be enough free volume and no Fermi liquids in the host medium — the reason why 'classical' positronium forms mainly in molecular crystals, amorphous materials, and

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polymers. The physics of Ps in such materials is reviewed in detail in Refs [1 – 7] (see also Refs [9 – 13]).

In metals, the strong multiparticle electron–positron interaction inhibits the formation of positronium, but if a metal has a cavity (a void), then the interaction of Ps localized in the cavity with electrons from outside it is to some extent suppressed. In this case, such an interaction occurs via the processes $\mathrm{Ps} \leftrightarrow \mathrm{e}^+ + \mathrm{e}^-$ [8], with the result that the cavity-localized positronium state is mixed (hybridized) with the conduction-band electron states and with the states of a positron localized in the same cavity. (This is akin to the state of a magnetic impurity hybridization with conduction-band electron states in the Anderson model [14].) As a result of this interaction, the average occupation number of the positronium level n_{Ps} turns out to be less than unity. We also note that the interaction due to the processes $\mathrm{Ps} \leftrightarrow \mathrm{e}^+ + \mathrm{e}^-$ is stronger than the relativistic intra-atomic interaction, ruling out the singlet–triplet classification for the states of such Ps. The annihilation lifetime of Ps becomes dependent on n_{Ps} in this case.

In the model under study, the average occupation number n_{Ps} of the positronium level is determined by the local density of states $\tilde{\rho}_{\mathrm{Ps}}(\omega)$,

$$n_{\mathrm{Ps}} = \int_{-\infty}^{+\infty} \tilde{\rho}_{\mathrm{Ps}}(\omega) f(\omega)\, \mathrm{d}\omega\,, \tag{1.1}$$

where $f(\omega)$ is the Fermi distribution function. By analogy with the behavior of a magnetic impurity in a normal Fermi liquid in the infinite-U Anderson model [15], it can be concluded that $\tilde{\rho}_{\mathrm{Ps}}(\omega)$ is two-peaked at low temperatures [8]. The lower and relatively broad peak is due to the virgin positronium state $\varepsilon_{\mathrm{Ps}}^0$ being hybridization-broadened — a phenomenon corresponding to the Anderson magnetic impurity model in its simplest version [14]. The second peak forms near the Fermi level, has its maximum at $\tilde{\rho}_{\mathrm{Ps}}(\omega)$, and corresponds to the so-called *Abrikosov-Suhl resonance* (also known as the *Kondo resonance*). The energy gap that forms in the superconducting state causes the dependence of $\tilde{\rho}_{\mathrm{Ps}}(\omega)$ on ω to change in the region where the resonance occurs. Thus, the temperature dependence of $\tilde{\rho}_{\mathrm{Ps}}(\omega, T)$ in the region $T \approx T_{\mathrm{c}}$ affects the dependence $n_{\mathrm{Ps}}(T)$ in this temperature region. In the actual system under consideration, the energy width 2Γ of the positronium level is much larger than the energy of the relativistic intra-atomic interaction. Thus, the two-quantum Ps annihilation involves multiple conversion of the spin state, with the result that the state of such interacting Ps is averaged over all four 1S states, one of which is a singlet and the three others are triplets. Because, further, the 2γ annihilation is only possible for parapositronium, the positronium lifetime in a cavity becomes $\tau_{\mathrm{Ps}} = 4 \times 125$ ps $= 500$ ns instead of the usual parapositronium vacuum lifetime 125 ps. As a result, the total 2γ annihilation probability w_2 ($w_2 = \tau_2^{-1}$) of a microcavity-trapped positron is [8]

$$w_2 = n_{\mathrm{Ps}} w_{\mathrm{Ps}} + (1 - n_{\mathrm{Ps}})\, w_{\mathrm{p}}\,, \tag{1.2}$$

where $w_{\mathrm{Ps}} = \tau_{\mathrm{Ps}}^{-1}$, and the 2γ annihilation probability w_{p} for a cavity-trapped positron in the one-particle state, depends on the overlap of the positron and electron wave functions that partly penetrate the cavity. The effect of this overlap is enhanced by the attraction between these particles [4 – 7]. A one-particle positron trapped by a cavity is localized near the inner surface of the cavity.

An important positron-based technique for studying solids is to observe the lifetime of thermalized positrons. A point to note here is that the annihilation, i.e., the transformation of an electron–positron pair to electromagnetic γ quanta, occurs when the distance between these particles is of the order of the Compton wavelength $\hbar/(mc) \sim 10^{-10}$ cm, where m is the electron mass and c is the speed of light [16, 17]. As a result, the lifetime τ of a thermalized electron in a Fermi liquid is inversely proportional to the electron density n_{e} at the point of location of the positron. As shown by Dirac [18], the 2γ annihilation probability $w = \tau^{-1}$ for a positron in such a system is

$$w = \pi r_0^2 c n_{\mathrm{e}}\,, \tag{1.3}$$

where $r_0 = e^2/(mc^2)$ is the classical electron radius. The quantity n_{e} depends on the concentration of fermions in the Fermi liquid and the attractive interaction between the positron and the electron environment. This last factor increases n_{e} considerably compared to that in a system of free particles.

Experiments in studies of the lifetime of thermalized positrons in solids show that τ_2 generally has a spectrum of values (or components), each one corresponding to the lifetime of a positron in a specific (say, ith) state. For a perfect, defect-free single crystal, there exists only one component, τ_1, which is the lifetime of a thermalized positron traveling freely through the crystal. Crystal lattice defects such as dislocations, vacancies, and microcavities have the capability to trap electrons, essentially because a trapped positron is localized farthest from the atomic nuclei in the crystal. In some cases, microscopic complexes of impurity atoms have positron trapping capabilities [19]. The lifetime of a trapped positron is specific to each type of defect.

In a real experiment, the resolving power of the apparatus puts a limit on how many components of the positron lifetime spectrum can be determined. Studies of ceramic high-temperature superconductors generally reveal three components, τ_1, τ_2, and τ_3, which, in that order, correspond to delocalized positrons, positrons trapped by lattice defects, and orthopositronium that forms in relatively large cavities. Because of the pick-off annihilation, the value of τ_3 is somewhat reduced compared to free orthopositronium. In cases of positronium formed in microcavities in HTSCs, $\tau_2 \sim (350-450)$ ps. We note that in normal metals, with microcavities produced at sizes of tens of angstroms, the measured τ_2 approaches 500 ps [5, 7]. This result agrees with Eqn (1.2).

Equation (1.2) also implies a relation between τ_2 and n_{Ps}, allowing data on the behavior of $\tau_2(T)$ to be used to draw conclusions on how the electronic structure of the material depends on temperature. Ceramic materials, with their high concentration of microcavities, have a very large τ_2 component.

This paper summarizes and interprets experimental results on $\tau_2(T)$ for HTSC samples of $(\mathrm{Bi,Pb})_2\mathrm{Sr}_2\mathrm{Ca}_2\mathrm{Cu}_3\mathrm{O}_x$ ((Bi,Pb)-2223) in the temperature range $T \sim T_{\mathrm{c}}$. These data are of interest for understanding the nature of the pseudogap that forms in undoped samples of an HTSC at $T > T_{\mathrm{c}}$ [20 – 26]. For some authors [24 – 30], the pseudogap is a precursor of the superconducting phase and a state-to-state transformation is a continuous process, while for others [31 – 36], there is only an indirect relation between the pseudogap and superconductivity.

In this paper, the model of interacting Ps localized in a cavity in an HTSC is used to interpret the behavior of $\tau_2(T)$ in the region $T \sim T_c$. It is assumed that in the pseudogap state, the system contains free fermions and a Bose gas of fermion pairs. The model of superconductivity used is three-dimensional, with electrons interacting via a contact attraction potential.

2. Experiment

Understanding the effect of superconductivity on the annihilation of positrons is not a new problem. Even as early as the 1950s, the time of the first experiments on positron annihilation in solids, attempts were made to use this method to study the phenomenon of superconductivity [37]. The hope was to observe directly how the onset of the superconducting state changes the electronic structure of a metal. This hope was not to be realized, however, because for classical superconductors, the changes sought (in the temperature range of interest) are too small to be observed this way. The advent of high-temperature superconductivity changed the situation and rekindled interest in the subject [37–79]. A number of early results on the effect of the superconducting state on positron annihilation in high-temperature superconductors are summarized by the present author elsewhere [37].

Experimental studies of the temperature dependence of the spectra of positronium lifetime components by various authors show that at temperatures close to T_c, under the transition to the superconducting state, the value of the defect-associated component τ_2 decreases [38–44, 55–59, 76–79]. The values of τ_1 and τ_2 obtained by various authors for (Bi,Pb)-2223 samples at temperatures around T_c are summarized in the Table.

The most definitive results on this effect were those from ceramic samples of (Bi,Pb)-2223 [59, 72]. Figure 1 plots the temperature dependence of two components of the positron lifetime spectrum, τ_1 and τ_2, obtained for (Bi,Pb)-2223 near $T_c = 105$ K [59]. Also shown is the temperature dependence of the electric resistance, $R(T)/R$ ($T \approx 300$ K), which characterizes the transition of the sample to the superconducting state.

The component $\tau_1 \approx 220$ ps is the lifetime of delocalized positrons; its intensity is $I_1 \approx 75\%$ according to the data in Ref. [59]. As seen from Fig. 1, τ_1 shows little or no temperature dependence in the neighborhood of T_c. A possible explanation is that the probability density of spatial localization of a positron in a state corresponding to the Bloch function overlaps only weakly with the superconducting CuO_2 planes [80, 81].

Table. Components τ_1 and τ_2 of the positronium lifetime spectrum at $T = T_c$ for Bi-2223 and (Bi, Pb)-2223 samples. Data from various sources.

Sample	τ_1, ps	τ_2, ps*	References
Bi-2223	230	396 (7%)	[62]
Bi-(2212 + 2223)	210	400	[70]
(Bi,Pb)-2223	221	420 (26%)	[59]
(Bi,Pb)-2223	193	359 (10%)	[72]
(Bi,Pb)-2223	200	310 (20%)	[66]
(Bi,Pb)-2223	200	540 (80%)	[60]
(Bi,Pb)-2223	195	373 (31%)	[99]

* Percent values in parentheses are the intensities of the τ_2 component.

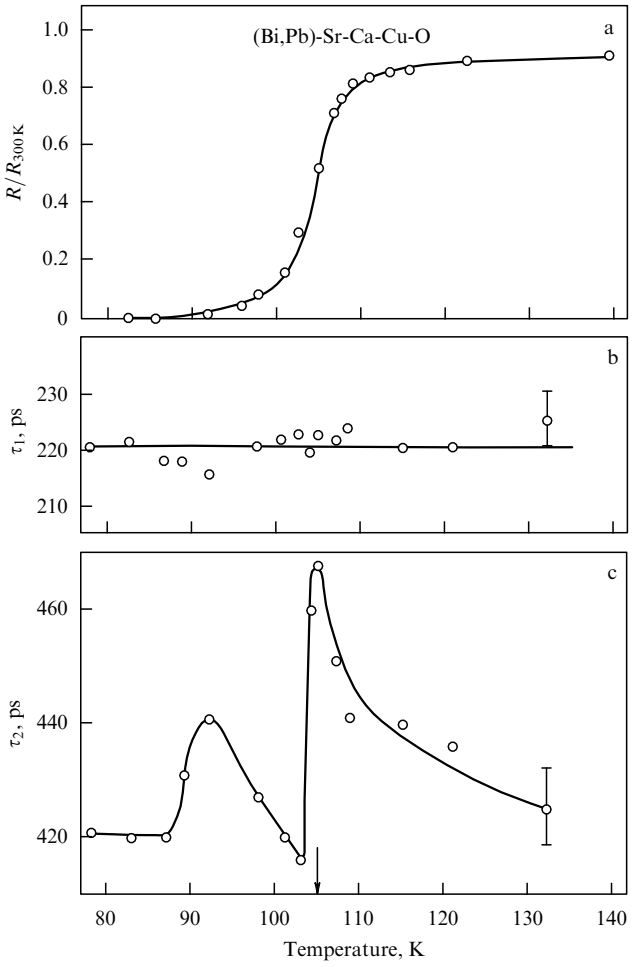

Figure 1. Physical properties vs temperature at around T_c for (Bi,Pb)-2223: (a) electric resistance $R(T)/R$ (300 K); (b) the lifetime of delocalized positrons $\tau_1(T)$; (c) the lifetime of cavity-trapped positrons $\tau_2(T)$. The arrow indicates T_c [59].

The effect of superconductivity on positron annihilation in a homogeneous Fermi liquid was studied theoretically in Refs [82–88].

The component τ_2 of the lifetime spectrum corresponds to positrons trapped by microcavities. The data in Fig. 1 on the temperature dependence of τ_2 near T_c was confirmed in Ref. [72]. The results for (Bi,Pb)-2223 in [72] are shown in Fig. 2.

The τ_2 versus T curves shown in Figs 1 and 2 point to a relation between τ_2 and the processes occurring in the electronic structure of an HTSC in the neighborhood of T_c. Decreasing the temperature in the range $\approx(105–150)$ K causes a decrease in $\tau_2(T)$. This temperature range is the one where the pseudogap forms. The transition to the superconducting state causes a decrease in τ_2 at $T = T_c$, indicating that the transition from the psedogap state to the superconducting state involves a sudden change in the electronic structure of the HTSC. We note that the general behavior of $\tau_2(T)$ near T_c does not correspond to a relatively smooth electric resistance R versus T curve in the same temperature region. According to experiments [26], electron photoemis-

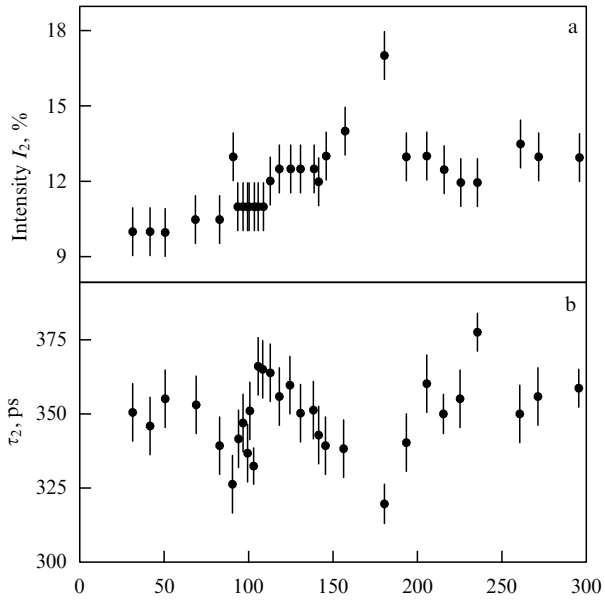

Figure 2. Results of the $\tau_2(T)$ component of the positron lifetime spectrum showing (a) its intensity $I_2(T)$ and (b) its magnitude as functions of temperature for (Bi,Pb)-2223 [72].

sion from HTSCs also undergoes changes in the T_c region under the superconducting transition, indicating, together with the preceding facts, that the temperature dependence of τ_2 is quite an informative effect as regards the electronic structure changes near T_c.

Hence, the τ_2 versus T dependence in pseudogap states is a new effect due to the nature of these states in high-temperature superconductors.

The second maximum, 92 K (see Fig. 1), is due to the $\approx 20\%$ presence of the (Bi,Pb)-2212 phase in the sample. The behavior of $\tau_2(T)$ observed near $T_c = 92$ K in the (Bi,Pb)-2212 phase is similar to that near $T_c = 105$ K for (Bi,Pb)-2213.

We note that data from various studies on the Bi-2223 and (Bi, Pb)-2212 phases show some sample-to-sample scatter in the value of τ_2 near T_c for the same composition (see the Table). The reason for this most likely relates to sample preparation techniques. Undoubtedly, the positron lifetime in a cavity in an HTSC depends on the size of the cavity [89 – 91], and samples prepared in various laboratories may vary in the average cavity size. The average occupation number of the Ps level $n_{Ps} \to 1$ with increasing the cavity size; however, for $\tau_2 \approx 500$ ps, it follows from Eqn (1.2) that due to the interaction of Ps with its environment, the spin of the Ps electron flips many times within the parapositronium annihilation lifetime of 125 ps. Experimental studies [5, 93 – 98] support the predicted existence of the limiting τ_2 value of 500 ps for positrons trapped by relatively large metal cavities.

Experiment shows that the spectrum of τ contains a component $\tau_3 \approx 1200$ ps of low intensity ($I_3 \approx 1\%$) [59], which corresponds to positronium that forms in an extended cavity and interacts weakly with the environment.

In summary, experimental results show that positronium localized in cavities with a size around 10 Å is in different states depending on whether the material is a metal or an insulator. For an insulator, localized positronium interacts relatively weakly with the environment and therefore preserves its basic properties as related to and determined by the intra-atomic relativistic interaction. In the case of a metal, however, the positronium–environment interaction is stronger than the intra-atomic relativistic interaction, leading to considerable changes in the basic properties of Ps and hence establishing a relation between these properties and the metal electronic structure.

3. Theory

3.1 Model

We list the key factors underlying the theoretical interpretation of the τ_2 versus T dependence in the neighborhood of T_c for ceramic HTSCs [8, 115].

(1) A positron trapped by a microcavity forms a positronium atom.

(2) The interaction of cavity-localized positronium with its electron environment occurs via the processes $Ps \leftrightarrow e^+ + e^-$, which are the hybridization of Ps states with the states of conduction-band electrons and with the one-particle state of the positron localized in the same cavity.

(3) This phenomenon is treated using the infinite-U Anderson model for a magnetic impurity in a normal Fermi liquid in the Kondo limit, that is, under the condition $\varepsilon_F - \varepsilon_d \gg \Gamma$, where ε_d is the impurity level energy and Γ is the 'hybridization width.'

(4) The effect of hybridization is a much stronger interaction compared to the relativistic intra-atomic interaction in Ps in the vacuum. The strength of this interaction is characterized by Γ.

Describing states of Ps in a metal cavity requires considering individual energy levels that characterize the system. The vacuum ground state energy ε^0_{Ps} of Ps relative to the energy of Ps component particles at rest is -6.8 eV. If cavity-localized Ps is regarded as a particle in a spherically symmetric potential well, then the ground state characterizing its motion is the 1s state [100]. The energy ε'_{Ps} of such Ps includes the energy ε_{1s} of the spatial localization of positronium within the spherical cavity, i.e., $\varepsilon'_{Ps} = \varepsilon^0_{Ps} + \varepsilon_{1s}$. The other parameters of the system are ε_p, the energy of the one-particle positron state in the cavity ($\varepsilon_p < 0$), and μ, the electron chemical potential in the metal. Figure 3 qualitatively illustrates the relative positions of these quantities.

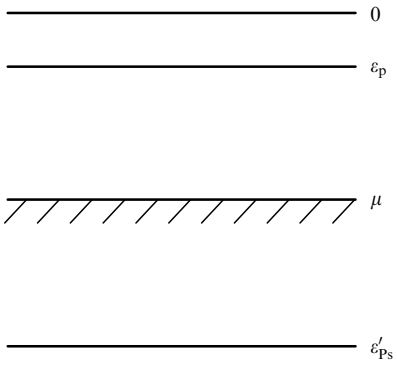

Figure 3. Schematic diagram of the energy levels ε'_{Ps}, ε_p, and μ, where $\varepsilon'_{Ps} = \varepsilon^0_{Ps} + \varepsilon_{1s}$ is the ground state energy of positronium localized in a spherical microcavity; ε^0_{Ps} is the binding energy ($= 6.8$eV) of the free 1S positronium atom; ε_{1s} is additional energy due to the localization of positronium in a spherical microcavity (1S state of the localized particle); ε_p is the energy of the one-particle state ($\varepsilon_p < 0$) of a positron localized in a microcavity; μ is the chemical potential of conduction band electrons [8].

A positron in a one-particle state in a metal microcavity is localized near the inner surface of the cavity. This phenomenon is due to the interaction of the positron with the electron environment, which surrounds and partly penetrates the cavity [4–7, 89–91, 101–104]. As a result of this interaction, the positron energy ε_p becomes negative relative to the energy of a positron at rest in the vacuum.

3.2 Hamiltonian

In accordance with the model outlined above, the following Hamiltonian is taken to describe the normal state of the system being considered [8]:

$$H = \sum_{\mathbf{k},\sigma} (\mu + \varepsilon_k)\, c^+_{\mathbf{k}\sigma}\, c_{\mathbf{k}\sigma} + \sum_{\beta} \varepsilon_p\, b^+_\beta b_\beta + \sum_{\sigma,\beta} \varepsilon'_{Ps}\, d^+_{\sigma\beta}\, d_{\sigma\beta} + V \sum_{\mathbf{k},\sigma,\beta} (c^+_{\mathbf{k}\sigma}\, b^+_\beta\, d_{\sigma\beta} + \text{h.c.})\,, \tag{3.1}$$

where μ is the chemical potential of the conduction-band electrons (see Fig. 3), $\varepsilon_k = E_k - E_{k_F}$, where $E_k = \hbar^2 k^2/(2m)$, and k_F is the absolute value of the electron Fermi wave vector. The operator $c^+_{\mathbf{k}\sigma}$ is the creation operator for a conduction band electron with wave vector $\mathbf{k}$ and spin defined by σ.

The second term in Eqn (3.1) is the energy operator for a cavity-trapped positron, and b^+_β creates a cavity-localized energy-ε_p spin-β positron. The energy ε_p includes the Coulomb and correlation interactions of the positron with electrons that penetrated the cavity.

The third term is the contribution from a cavity-localized 1S-state Ps atom, $\varepsilon'_{Ps} = \varepsilon^0_{Ps} + \varepsilon_{1s}$, where $\varepsilon^0_{Ps} = -6.8$ eV is the ground state energy of Ps relative to e^+ and e^- at rest and ε_{1s} is the contribution to the energy of Ps due to its being localized in a spherically symmetrical cavity. The subscript 1s characterizes the ground state of the particle (positronium) that arises due to its localization in a spherical cavity.

Hamiltonian (3.1) implies that the relativistic intra-atomic interaction in the positronium atom is negligible compared to the positronium energy level width 2Γ that arises due to the processes $Ps \leftrightarrow e^+ + e^-$. Accordingly, a bosonic operator is assumed to create positronium with definite values of the electron and positron spins [100].

The fourth term in Hamiltonian (3.1), the interaction operator H_{int}, arises due to the hybridization of the state of Ps with the states of conduction-band electrons and with the state of the cavity-localized positron. All matrix elements for this process are taken to be equal to a constant V.

3.3 State hybridization

The annihilation lifetime τ_2 of a microcavity-trapped positron depends on the average occupation number of the positronium state n_{Ps} (see Eqn (1.2)). It follows from the form of Hamiltonian (3.1) that the method developed for describing a magnetic impurity in a normal metal [15, 105, 106] can be used to determine n_{Ps}. For this, we consider the temperature-dependent correlation Green's function

$$\widetilde{G}_{Ps,\sigma}(t_1 - t_2) = -\mathrm{i}\theta(t_1 - t_2) \times \langle F_\sigma(t_1)\, F^+_\sigma(t_2) + F^+_\sigma(t_2)\, F_\sigma(t_1)\rangle\,, \tag{3.2}$$

where the function $\theta(t_1 - t_2) = 1$ for $t_1 > t_2$ and is zero for $t_1 < t_2$. The symbol $\langle \ldots \rangle$ denotes averaging over the Gibbs distribution.

$$F_\sigma(t) = B^+_p D_{Ps,\sigma}(t)\,. \tag{3.3}$$

The operators $B^+_p(t)$ and $D_{Ps,\sigma}(t)$ are defined as

$$B^+_p(t) = \exp(\mathrm{i}H't)\, b^+ \exp(-\mathrm{i}H't)\,, \tag{3.4}$$

$$D_{Ps,\sigma}(t) = \exp(\mathrm{i}H't)\, d_\sigma \exp(-\mathrm{i}H't)\,,$$

where

$$H' = H - \mu\widehat{N}_e - (\mu + \varepsilon_p) \sum_{\sigma,\beta} d^+_{\sigma\beta}\, d_{\sigma\beta} - \sum_\beta \varepsilon_p\, b^+_\beta b_\beta\,. \tag{3.5}$$

The Hamiltonian H in Eqn (3.5) is given by (3.1) and $\widehat{N}_e$ is the number operator for conduction-band electrons. The system contains only one positron, and because the Hamiltonian suboperators do not change the positron spin state, the spin indices are omitted for B^+_p and b^+.

Transformations (3.4) and (3.5) for the original positron (b_β) and positronium ($d_{\sigma\beta}$) operators involved in Hamiltonian (3.1) enable using the well-known Anderson magnetic impurity model in handling the problem.

According to Eqn (1.1), the quantity n_{Ps} is determined by the local density of states $\tilde{\rho}_{Ps}(\omega)$, which is given by

$$\tilde{\rho}_{Ps}(\omega) = -\frac{1}{\pi}\,\mathrm{Im} \sum_\sigma \widetilde{G}_{Ps,\sigma}(\omega)\,. \tag{3.6}$$

To the operators $D_{Ps,\sigma}$ and B_p there correspond the single-particle propagators

$$G_{Ps,\sigma}(\omega + \mathrm{i}0) = \left[\omega - \varepsilon_{Ps} - \sigma_{Ps,\sigma}(\omega + \mathrm{i}0)\right]^{-1}, \tag{3.7}$$

where $\varepsilon_{Ps} = \varepsilon^0_{Ps} + \varepsilon_{1s} - \mu - \varepsilon_p$, and

$$G_p(\omega + \mathrm{i}0) = \left[\omega - \sigma_p(\omega + \mathrm{i}0)\right]^{-1}. \tag{3.8}$$

The 'noncrossing' expressions for the eigenenergies of positronium, $\sigma_{Ps\sigma}$, and the positron, σ_p, take the following form when the Fermi liquid surrounding the cavity is in the normal state:

$$\Sigma_{Ps}(\omega + \mathrm{i}0) = V^2 \sum_{\mathbf{k}} \left(1 - f(\varepsilon_k)\right) G_p(\omega - \varepsilon_k + \mathrm{i}0)\,, \tag{3.9}$$

and

$$\sigma_p(\omega + \mathrm{i}0) = 2V^2 \sum_{\mathbf{k}} f(\varepsilon_k)\, G_{Ps}(\omega + \varepsilon_k + \mathrm{i}0)\,, \tag{3.10}$$

where $f(\varepsilon_k)$ is the Fermi distribution function, ε_k is the kinetic energy of a conduction-band electron measured from the chemical potential μ, and the electron spin index σ is omitted. The summation in Eqn (3.10) ranges over spin states.

The functions G_{Ps} in (3.7) and G_p in Eqn (3.8), with σ_{Ps} and σ_p substituted from Eqns (3.9) and (3.10), fully correspond to the two propagators that are introduced for describing the properties of a magnetic impurity [15].

Introducing the functions G_{Ps} and G_p allows finding the correlation function $\widetilde{G}_{Ps}$. In the Matsubara representation, where $\widetilde{G}_{Ps}(\mathrm{i}\omega_n)$ is a function of discrete 'frequencies' ω_n, we have [15]

$$\widetilde{G}_{Ps}(\mathrm{i}\omega_n) = \frac{1}{Z} \int_C \frac{\mathrm{d}l}{2\pi\mathrm{i}} \exp(-\beta l)\, G_p(l)\, G_{Ps}(l + \mathrm{i}\omega_n)\,, \tag{3.11}$$

where $\beta = (kT)^{-1}$; the contour C runs counterclockwise and encloses all singularities of the integrand; Z is the partition

function,

$$Z=\int_{-\infty}^{+\infty}\exp\left(-\beta\varepsilon\right)\left[\rho_{\mathrm{p}}(\varepsilon)+\rho_{\mathrm{Ps}}(\varepsilon)\right]\mathrm{d}\varepsilon\,, \tag{3.12}$$

where

$$\rho_{\mathrm{p}}(\varepsilon)=-\pi^{-1}\,\mathrm{Im}\,G_{\mathrm{p}}(\varepsilon+\mathrm{i}0)\,,$$

$$\rho_{\mathrm{Ps}}(\varepsilon)=-\pi^{-1}\,\mathrm{Im}\sum_{\sigma}G_{\mathrm{Ps},\,\sigma}(\varepsilon+\mathrm{i}0)\,.$$

It follows from Eqn (3. 11) for $\widetilde{G}_{\mathrm{Ps}}(\mathrm{i}\omega_n)$ and from definition (3.6) of $\rho_{\mathrm{Ps}}(\omega)$ that [15]

$$\tilde{\rho}_{\mathrm{Ps}}(\omega)=\frac{1}{Z}\left[1+\exp\left(-\beta\omega\right)\right]\int_{-\infty}^{+\infty}\exp\left(-\beta\varepsilon\right)\times\rho_{\mathrm{p}}(\varepsilon)\,\rho_{\mathrm{Ps}}(\varepsilon+\omega)\,\mathrm{d}\varepsilon\,. \tag{3.13}$$

3.4 Effect of the superconducting state on Ps

As noted in the Introduction, $\tilde{\rho}_{\mathrm{Ps}}(\omega)$ has a Kondo peak near the Fermi level in the normal Fermi liquid state. The energy gap 2Δ that occurs in the fermion spectrum in the superconducting state drastically affects the behavior of $\tilde{\rho}_{\mathrm{Ps}}(\omega)$ in the region $|\omega|\sim\Delta$. In the superconducting case, with the formation of new fermions taken into account [107], the eigenenergies σ_{Ps} and σ_{p} are given by [8]

$$\sigma_{\mathrm{Ps}}(\omega+\mathrm{i}0)=V^2\sum_{\mathbf{k}}\left[u_k^2 f(-\eta_k)\,G_{\mathrm{p}}(\omega-\eta_k+\mathrm{i}0)+v_k^2 f(\eta_k)\,G_{\mathrm{p}}(\omega+\eta_k+\mathrm{i}0)\right], \tag{3.14}$$

$$\sigma_{\mathrm{p}}(\omega+\mathrm{i}0)=2V^2\sum_{\mathbf{k}}\left[u_k^2 f(\eta_k)\,G_{\mathrm{Ps}}(\omega+\eta_k+\mathrm{i}0)+v_k^2 f(-\eta_k)\,G_{\mathrm{Ps}}(\omega-\eta_k+\mathrm{i}0)\right], \tag{3.15}$$

where, according to the Bardeen – Cooper – Schrieffer (BCS) theory,

$$\eta_k=\sqrt{\varepsilon_k^2+\Delta^2}\,,\quad u_k^2=\frac{1}{2}\left(1+\varepsilon_k\eta_k^{-1}\right),\quad v_k^2=\frac{1}{2}\left(1-\varepsilon_k\eta_k^{-1}\right).$$

In the interval $-\Delta<\omega<\Delta$, $\mathrm{Im}\,\sigma_{\mathrm{Ps}}(\varepsilon_{\mathrm{Ps}}+\omega)$ and $\mathrm{Im}\,\sigma_{\mathrm{p}}(\varepsilon_{\mathrm{Ps}}+\omega)$ can be considered zero, and the dependence of $\mathrm{Re}\,\sigma_{\mathrm{Ps}}(\varepsilon_{\mathrm{Ps}}+\omega)$ on ω neglected. With this in mind, for ω within the gap, we have

$$\tilde{\rho}_{\mathrm{Ps}}(\omega)=2\delta\left[\varepsilon_{\mathrm{Ps}}-\omega-\mathrm{Re}\,\sigma_{\mathrm{p}}(\varepsilon_{\mathrm{Ps}}-\omega)\right], \tag{3.16}$$

and

$$\mathrm{Re}\,\sigma_{\mathrm{p}}(\varepsilon_{\mathrm{Ps}}-\omega)=2V^2\left(\int_{-D}^{-\Delta}\frac{N(\varepsilon)f(\varepsilon)}{\varepsilon-\omega}\,\mathrm{d}\varepsilon+\int_{\Delta}^{D}\frac{N(\varepsilon)f(\varepsilon)}{\varepsilon-\omega}\,\mathrm{d}\varepsilon\right), \tag{3.17}$$

where $2D$ is the conduction band width.

According to the BCS theory,

$$N(\varepsilon)=\begin{cases}\dfrac{|\varepsilon|\,N_0}{\sqrt{\varepsilon^2-\Delta^2}}\,, & |\varepsilon|>\Delta\,,\\ 0\,, & -\Delta<\varepsilon<\Delta\,.\end{cases} \tag{3.18}$$

in the superconducting state. The one-spin density of states in the normal-state conduction band is taken to be equal to the constant N_0.

Experimental data on HTSCs show that for $T=T_{\mathrm{c}}$, the quantity $\Delta(T_{\mathrm{c}})$ (hereafter denoted simply by Δ) remains constant and greatly exceeds T_{c} [27, 108, 109], and hence if ω is within the gap and $\omega\to-\Delta$, then the right-hand side of Eqn (3.17) is correctly truncated to its first term (in which $f(\varepsilon)\to1$). As a result, the integration in Eqn (3.17) can be done analytically. The contribution to n_{Ps} from the integration of the δ-function defined by (3.16) is

$$\delta n_{\mathrm{Ps}}=\left[\left|-1-\frac{\partial}{\partial\omega}\,\mathrm{Re}\,\sigma_{\mathrm{p}}(\varepsilon_{\mathrm{Ps}}-\omega)\right|_{\omega=\omega_0}\right]^{-1}, \tag{3.19}$$

where ω_0 ($\omega_0>-\Delta$) is the value of ω at which the argument of the δ-function in Eqn (3.16) vanishes. If $|\varepsilon_{\mathrm{Ps}}|\gg\Delta$ and $|\varepsilon_{\mathrm{Ps}}|\gg\Gamma$, then ω_0 is found from the equation $\varepsilon_{\mathrm{Ps}}-\omega+2\Gamma\Delta(\sqrt{\Delta^2-\omega^2}\,)^{-1}=0$.

We note, however, that the weight of the ω_0 peak is negligible because for the superconducting state, $N(\varepsilon)$ depends on ε in accordance with (3. 18) (Fig. 4). The value of n_{Ps} due to this peak is of the order of $\Gamma^2\Delta/|\varepsilon_{\mathrm{Ps}}|^3\ll1$, where $\Gamma=V^2N_0$ is the hybridization width.

Outside the gap, as $\omega\to-\Delta$, $\tilde{\rho}_{\mathrm{Ps}}(\omega)\to0$ because $N(\omega)\to\infty$ in this region. Numerical calculations [8] show that in the superconducting state, for $+\Delta$ outside the gap close to $\tilde{\rho}_{\mathrm{Ps}}(\omega)$, the contribution to n_{Ps} is also negligible. Therefore, close to $\omega=\pm\Delta$, the fermion structure properties of the superconducting state do not make a large additional contribution to n_{Ps}. However, because of the formation of the gap 2Δ, n_{Ps} does not receive a contribution of the Kondo peak produces in the normal state [8].

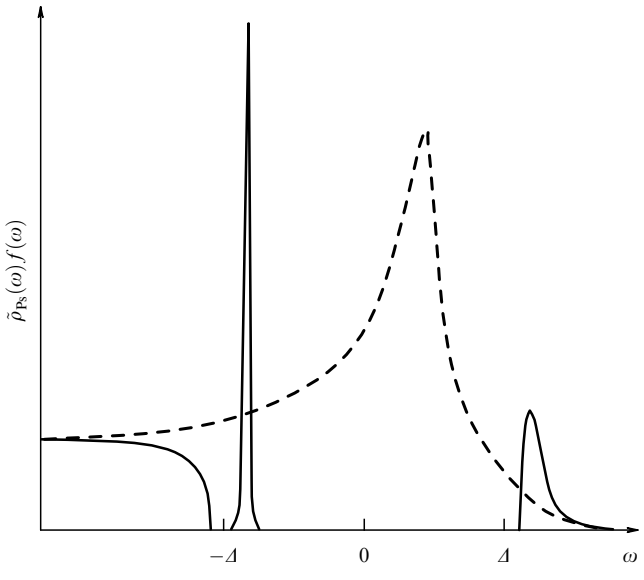

Figure 4. Schematic illustration of $\tilde{\rho}_{\mathrm{Ps}}(\omega)f(\omega)$ as a function of ω for the superconducting (solid line) and normal (dashed line) states in the limited range of ω around the energy gap. $\tilde{\rho}_{\mathrm{Ps}}(\omega)$ is the physical density of states for interacting positronium localized in a microcavity and $f(\omega)$ is the Fermi distribution function. The peak on the normal-state curve is due to the *Kondo resonance*. Experimental data [59, 72] suggest that at the superconducting-to-pseudogap transition at $T=T_{\mathrm{c}}$, there is a jump in the weight of the peak on the curve $\tilde{\rho}_{\mathrm{Ps}}(\omega)$ that arises in the superconducting phase inside the gap for $\omega\approx-\Delta$ [115].

3.5 Influence of the gap state on Ps

There is currently no generally accepted theory of the pseudogap in high-temperature superconductors. Some authors believe that this state involves the formation of excited Cooper pairs and free fermions [24]. In our view [115], the experimental $\tau_2(T)$ behavior of (Bi,Pb)-2223 near T_c [59, 72] can be interpreted by assuming that in the pseudogap state, as $T \to T_c$ ($T > T_c$), the fermion density of states is given by

$$N(\varepsilon) = \begin{cases} N_0, & |\varepsilon| > \Delta\,, \\ 0, & -\Delta < \varepsilon < \Delta\,. \end{cases} \tag{3.20}$$

Equation (3.20) is consistent with experimental data, which show that the width of the gap changes continuously under the transition from the superconducting to the pseudogap state [27, 108, 109]. Expression (3.20) implies the formation of an ultracold Bose gas of bound fermion pairs at $T > T_c$. Also, the use of Eqn (3.20) to determine $\rho_{Ps}(\omega)$ implies that these Bose pairs do not participate in the hybridization of the Ps state. With $N(\varepsilon)$ defined by Eqn (3.20), it follows from Eqn (3.17) that for ω within the gap,

$$\mathrm{Re}\,\sigma_p(\varepsilon_{Ps} - \omega) = 2\,\frac{\Gamma}{\pi}\ln\left(\frac{\omega + \Delta}{D}\right). \tag{3.21}$$

Expression (3.21) diverges logarithmically as $\omega \to -\Delta$. A similar result arises in the infinite-U Anderson model for a magnetic impurity in a normal metal at low temperatures. In this model, it is known that the logarithmic $T \to 0$ divergence results in the local density of states of a magnetic impurity showing a Kondo resonance at a certain value $\omega - T_0$, where $T_0 > 0$. It follows from Eqns (3.16) and (3.21) that in the system under study, $\tilde{\rho}_{Ps}(\omega)$ has a peak at $\omega = -\Delta + T_0$, where T_0 is determined from the equation

$$\varepsilon_{Ps} + \Delta - T_0 = \frac{2\Gamma}{\pi}\ln\left(\frac{T_0}{D}\right). \tag{3.22}$$

From Eqn (3.19), the change in n_{Ps} is then given by

$$\delta n_{Ps} = \left[1 + \frac{2}{\pi}\,\frac{\Gamma}{T_0}\right]^{-1}. \tag{3.23}$$

Thus, the peak in $\tilde{\rho}_{Ps}(\omega)$ that arises in the superconducting phases inside the gap at ω close to $-\Delta$ (see Fig. 4) exhibits a jump-like increase in weight to $\approx \pi T_0/(2\Gamma)$ due to the formation of a pseudogap at $T = T_c$.

Experimental results for (Bi,Pb)-2223 [59, 72] show that in a relative expression, the jump in $\tau_2(T)$ at $T \approx T_c$ that occurs due to the transition from the superconducting to pseudogap state is $\delta\tau_2/\tau_2 \sim 0.1$, which can be compared with the values $\delta\tau_2/\tau_2$ determined by Eqn (1.2). If $\tau_2 \approx 500$ ps, then from Eqn (1.2) with $w_{Ps} = 500^{-1}$ ps^{-1} and $w_p = 250^{-1}$ ps^{-1} [78, 98, 110, 111], it follows that

$$\frac{\delta\tau_2}{\tau_2} \simeq \delta n_{Ps}\,. \tag{3.24}$$

In accordance with Eqn (3. 24), this gives $T_0 \sim 0.1\Gamma$.

4. Conclusion

By modeling Ps that forms in a microcavity in an HTSC and interacts with its surroundings via the Ps $\leftrightarrow e^+ + e^-$ processes, it is possible to link experimental results with the theory of the electronic structure that forms in a superconductor in the T_c region. The jump discontinuity in $\tau_2(T)$ observed in HTSCs at $T = T_c$ relates to the change in the Kondo state of positronium.

In a superconductor, Cooper pairs form a condensate, and according to the BCS theory, the fermion density of states $N(\varepsilon)$ is given by Eqn (3.18). As a result, the Kondo peak that forms on the $\tilde{\rho}_{Ps}(\omega)$ curve has a vanishingly small weight. In the pseudogap state, bound fermion pairs form an 'ultracold' Bose gas [114]. Experimental results [59, 72] on $\tau_2(T)$ in the vicinity of T_c can be interpreted by assuming that for $T > T_c$, bound fermion pairs take no part in the hybridization of the Ps state. It then follows from Eqn (3.20) for $N(\varepsilon)$ that under the superconducting-to-pseudogap transition, the weight of the Kondo peak that forms on the $\tilde{\rho}_{Ps}(\omega)$ curve increases by a jump. Above T_c, as the temperature increases, the bosons made of fermion pairs are gradually destroyed, and the concentration of free fermions correspondingly increases [28, 112–115]. As a result, in the pseudogap temperature region, increasing T leads to a decrease in $\tau_2(T)$.

In conclusion, effects due to the formation of positronium in metal cavities offer a useful tool to study the electronic structure of metals.

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