How long it takes para-positronium *and* ortho-positronium to become para-positronium *or* ortho-positronium? Decoherence of positronium in a matter

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Abstract

Because of small gap between the energy of para-positronium (p-Ps) and ortho-positronium (o-Ps) it was assumed the possibility of the existence of superposition of p-Ps and o-Ps states as a result of formation of positronium (Ps) from pre-Ps terminating in a free volume of matter. Then it was assumed the interaction hamiltonian for Ps and the matter from the wall of the free volume and the time evolution of the system was calculated. It was shown that the superposition of Ps states decohere in the basis of p-Ps and o-Ps and the decoherence time was estimated. Due to this there was motivated that the correction in decomposition of the spectra measured by the positron annihilation lifetime spectroscopy (PALS) ought to be done.

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I.   INTRODUCTION

The most powerful model of formation of the positronium atom in the matter comes from Stepanov and Byakov [1]. A positron from the irradiation source (the kinetic energy of positron produced by the most exploited isotope ^{22}Na [2] is less than 0.5 MeV) passing through the sample produces a set of ions while its energy is loosing. Due to this model, at first, each of electrons caused by ionization receives about 1 keV of the kinetic energy and is able to ionize other particles. Further ionizations release 30-100 eV each and produce next charged particles which form clusters called *spurs*. If the energy of the positron decreases to about 1 keV the ionization regions go less distant and overlap each other. Finally the positron ends up in the spreading cloud of ionized particles called *blob* with the energy lower than the ionization level. Further lose of energy of positron is consumed at most by vibrations of molecules and at about the thermalization level of energy the production of positronium atom arises as a profitable process.

Before the formation of positronium atom, an interacting positron and an electron can leave the blob as a weakly interacting, unlocalized system (pre-Ps) and migrate to a near free volume forming the localized Ps. One believes that at this time the whole population of Ps consists of p-Ps (spin number $S=0$) and o-Ps ($S=1$) so the spin number for each particle is definite. Such a Ps can annihilate in different ways: 1). the annihilation of p-Ps releases two gamma quanta, 2). o-Ps releases three gamma quanta, 3). each Ps can annihilate with the electron captured from the environment (*pick-off* process). The probability of pick-off annihilation rises with the local density of electrons and dominates in the case of annihilation in a matter. In the case of o-Ps the annihilation via pick-off is two-quantum process. However if the free volume was not reached the positron annihilates as a quasi-free particle with one of electrons from the bulk (in particular those from the blob).

The most serviceable channel of annihilation of the positron in a matter to applied physics (and also the easiest to measure) is long-living o-Ps which had been succeeded in reaching the free volume and annihilating by pick-off. The most important to us is that, for refine the long living component from the lifetime spectra received from the spectrometer, the spectra have to be decomposed into elementary channels of annihilation (free positron annihilation, ortho- and para-Ps annihilation, etc.). Usually the exponential statistics of annihilation rate for each channel is assumed in order to decompose the PALS spectrum.

II.   THE MOTIVATION

The papers exploiting the blob model assume the definite value of spin number for pre-Ps; as an example see positronium formation formulas in [3]. However because the difference of energies of p-Ps and o-Ps states in the vacuum is about $8.4 \cdot 10^{-4}$ eV [4], one can expect that the spin quantity could change during the migration of a pre-Ps through the sample due to the intermolecular interactions. It seems to be no reason to consider only certain definite spin number, e.g. only o-pre-Ps. Instead of that one can suppose that quasi-free Ps enters a free volume as a mixture of para and ortho states and thus the spin number could not be a proper number for such initial state.

The value of spin of Ps plays the important role in further analysis of Ps life. The annihilation of Ps, as a electromagnetic process, should obey the principle of conservation of the parity number (here charge parity). This number for Ps in the ground state and the spin value S is $\pi_C = (-1)^S$ whereas for n photons is $\pi_C = (-1)^n$ [5]. So until the spin number is not well defined, the system cannot decay with the emission of any definite n photons. Thus supposing that Ps is the mixture of p-Ps and o-Ps after entering a free volume one could expect that Ps can "live" in the free volume without giving a decay signal until it becomes p-Ps *or* o-Ps. This implies that one cannot decompose the PALS spectra simply into the exponential curves for p-Ps and o-Ps because the decay statistics cannot start just after the birth of Ps. In our opinion as long as there exists the population of Ps which is a mixture of spins one should make the correction when decomposing the PALS spectra (the analysis of the correction way is not the subject of this paper). Here we show that it is expected theoretically to decohere Ps in the p-Ps and o-Ps basis and we estimate the time of decoherence.

III.   HOW LONG LASTS THE DECOHERENCE OF PS MIXTURE? THE METHOD OF CALCULATION

The most convenient hamiltonian to consider the spin system interacting with the environment of spins (*bath*) is the Heisenberg hamiltonian [6] which is the phenomenological expression incorporated an overlapping of wave functions of electrons of the system and an environment [7, 8]. The problem of the decoherence of certain spin systems, in particular

consisting of a pair of particles interacting with the bath, was considered in [9–11] which support our calculation method.

Consider the hamiltonian for interaction of Ps and the molecules from the wall of the free volume

$$H = J\frac{\hbar^2}{4} \sum_{i=3}^{N+2} \bar{\sigma}^{(2)} \circ \bar{\sigma}^{(i)}, \tag{1}$$

where J- coupling constant, $\sigma^{(2)}$- Pauli matrices for the electron in Ps, $\sigma^{(i)}$- Pauli matrices for the i-th (of N) electron from an environment, $\circ$- scalar product. Suppose the initial (just after the localization of Ps in the free volume) state of the whole system as $\rho_0 \equiv |\Psi_0\rangle\langle\Psi_0|$, where

$$|\Psi_0\rangle = |Ps\rangle_0 \prod_{i=3}^{N+2} |s_i\rangle \equiv |Ps\rangle_0|S\rangle \tag{2}$$

and

$$|Ps\rangle_0 = \frac{1}{2}(|0,0\rangle + |1,-1\rangle + |1,0\rangle + |1,+1\rangle). \tag{3}$$

The ket $|S\rangle$ denotes the state of electrons of the environment whereas the numbers in kets are s and s_z values for Ps respectively. The latest equation expresses the supposition that after many interactions with the bulk, the state of Ps, just after passed into the free volume, do not distinguish any particular Ps state.

The evolution in time gives the following expression for the whole state at t

$$\rho(t) = |\Psi_t\rangle\langle\Psi_t|, \tag{4}$$

where $|\Psi_t\rangle = e^{-iHt/\hbar}|\Psi_0\rangle$. For the positronium only, we calculate the state at t as

$$\rho_{Ps}(t) = Tr_{env}[\rho(t)] \tag{5}$$

tracing over the environmental space.

In order to estimate the admixture of p-Ps in o-Ps at t we can calculate nondiagonal elements of $\rho_{Ps}(t)$. More precisely we consider the expression

$$S(t) = \sum_{s_z=-1}^{+1} |\langle s=0|\rho_{Ps}(t)|s=1,s_z\rangle|^2 \tag{6}$$

which is expected to collapse with time. The time when it reaches the minimum value we define as the time of the decoherence, T_d.

Because of the mathematical problems with calculating whole $\rho(t)$ analytically we made the simplification

$$|\Psi_t\rangle = e^{-iHt/\hbar}|\Psi_0\rangle \simeq [1 + \ldots + \frac{1}{3!}(-\frac{itH}{\hbar})^3]|\Psi_0\rangle, \tag{7}$$
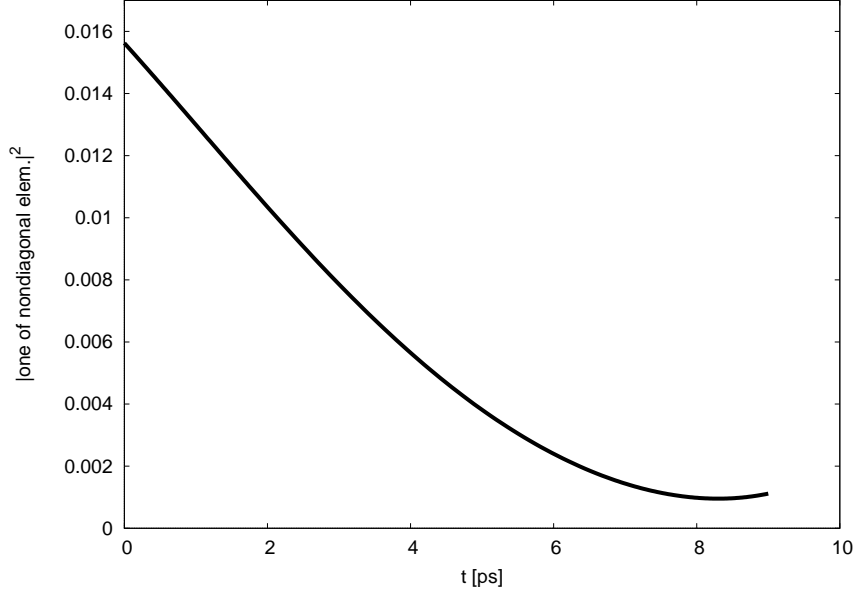
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FIG. 1. $|\rho_{[0,0;1,+1]}(t)|^2$ calculated for a random initial state vector (2). The interaction of Ps with $N=5$ electrons from the wall was assumed. The time for minimal value of the function is regarded as the decoherence time.

which still allows to approximate T_d correctly (see Appendix).

IV.   RESULTS AND DISCUSSION

The numerical calculations of (6) using (7) brings to the following statements:

1. One can observe indeed the decrease of $S(t)$ in the basis of p-Ps and o-Ps states (fig. 1), but nondiagonal terms do not disappear completely. Probably after the decrease of $S(t)$ shown in fig. 1, the oscillations could be obtained (that requires next expansion terms of the evolution operator) which would agree with the results of calculations of decoherence for other complex systems in the spin bath [10, 11]. T_d is about 10 ps which means that the effect of the existence of the mixture of states lasts the reasonable time for PALS experiments and one should take into account this effect by decomposing the PALS spectra. This result authors consider as the most significant result of this work.

2. Skipped powers of hamiltonian in the evolution operator do not affect substantially the value of the decoherence time (fig. 2). The figure compares the calculations with the 2-nd and the 3-rd power of H as a highest power. The minimum value of the curves in fig. 2 is
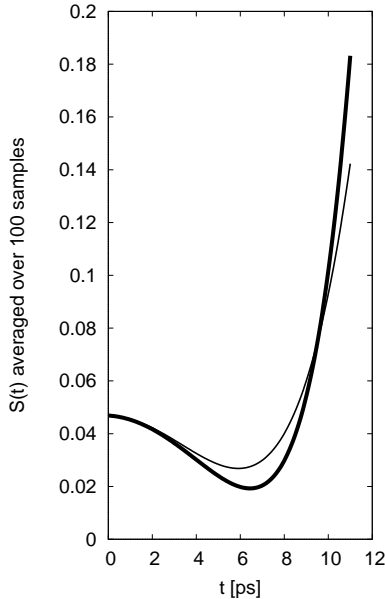
FIG. 2. $S(t)$ averaged over 100 randomly chosen samples of initial state vector for assumed N=7 electrons interacting with Ps atom. The comparison of calculations with truncation of the evolution operator by H^2 (thin line) and by H^3 (bold line).

stable and the area of divergence of both polynomials is for times exceeding T_d (the goal of this paper is to estimate T_d but not to calculate the time evolution of the system at any time. For extinguish the increasing value of both polynomials for rising time one need to calculate next powers of H in the expansion of the evolution operator which give higher powers of polynomials dominating at greatest values of t). The next terms of expansion may change $S(t)$ for greater values of time and thus may be an appropriate correction of T_d for slow decoherence (small number of electrons in the bath).

3. Decoherence time depends on a coupling constant J, which was set assuming that the energy of interaction of Ps and the electrons from the wall is about 10^{-4} eV (this is the energy which could convert ortho and para states and cause the initial mixture state. Such a value of energy for the interaction of Ps in the free volume is reasonable only for some specific cases, e.g. when ortho-para conversion takes place. This process is characteristic only for certain substances [12]). If the energy of the interaction has lower value one can expect that the decoherence time increases (e.g. if the interaction energy is set to 10^{-5} eV then T_d=70 ps).

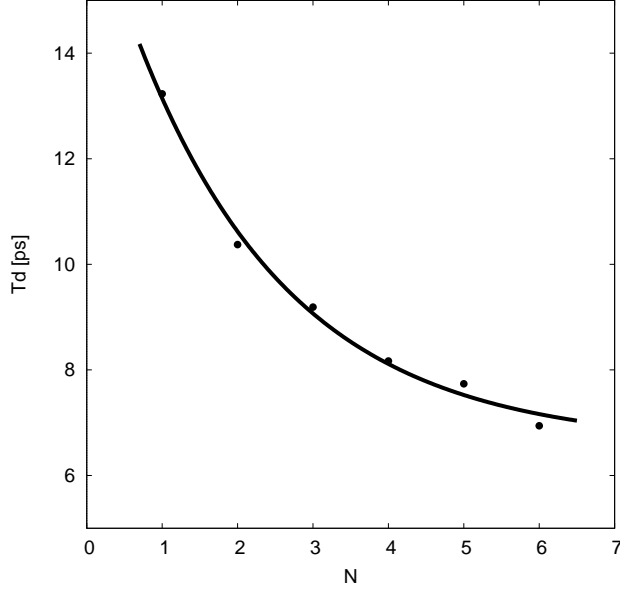4. The value of T_d decreases with the number N of electrons in the environment exponentially

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FIG. 3. The decoherence time T_d as a function of the number N of interacting electrons with Ps. The value is averaged over 100 randomly chosen initial state vectors. The points- the result of calculations, the line- the fitting curve.

(the fitting curve in fig. 3).

Furthermore the following observations seem to be relevant.

5. If one set in numerical calculations the magnetisation of the environment (all spins of the environment in the same direction) one turns out the suppression of the decoherence: it makes T_d shorter for given N and the minimum value of $S(t)$ becomes shallower, the more shallow the greater is N. This situation however cannot be treated as an numerical picture for the ferromagnetic sample. The ferromagnetic crystals do not form free volumes needed for Ps to be formed. Such property of the bath may be rather connected with the properties of some big molecules with the stable magnetization.

6. The Heisenberg hamiltonian leads to the reasonable results in the case of positronium decoherence problem but it shows that the decoherence is not complete in the basis p-Ps, o-Ps (there exist every time the population of Ps atoms in the mixed state). The interaction hamiltonian needs further studies and one can suspect that the incomplete decoherence is an artefact of the calculations with the use of too simple H (e.g. the constant value of the coupling constant in Heisenberg hamiltonian suggests the static picture of the interaction which seems to be simplified view of the real case).

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Appendix

Using the property of Pauli matrices

$$\sigma_i \sigma_j = \delta_{ij} \cdot 1 + i \sum_k \epsilon_{ijk} \sigma_k, \tag{A.1}$$

where ϵ_{ijk} is Levi-Civita symbol, one can reduce any n-th power of H down to the linear terms for each particle. One can check that any odd power n of (1) can be expressed as

$$\sum_{i,j,\ldots=3}^{N+2} \alpha_{ijk\ldots n} \cdot \sigma^{(2)} \circ \sigma^{(i)} \cdot \sigma^{(j)} \circ \sigma^{(k)} \cdot \ldots \cdot \sigma^{(n-1)} \circ \sigma^{(n)}, \tag{A.2}$$

whereas an even power n as

$$\sum_{i,j,\ldots=3}^{N+2} \beta_{ijk\ldots n-1} \cdot \sigma^{(2)} \circ \sigma^{(i)} \cdot \sigma^{(j)} \circ \sigma^{(k)} \cdot \ldots \cdot \sigma^{(n-2)} \circ \sigma^{(n-1)} +$$
$$+ \sum_{i,j,\ldots=3}^{N+2} \gamma_{ijkl\ldots n} \cdot \sigma^{(i)} \circ \sigma^{(j)} \cdot \sigma^{(k)} \circ \sigma^{(l)} \cdot \ldots \cdot \sigma^{(n-1)} \circ \sigma^{(n)}. \tag{A.3}$$

Some parts of the sums reduce (still using (A.1)) in particular to the most common (existing for any n and N) operator $\aleph(n, N) \cdot \sigma^{(2)} \circ \sigma^{(i)}$, where the coefficient $\aleph(n, N)$ is the exponential function of n and linearly dependent on N (e.g. for $N=2$ its value is $1/3 \cdot 2^{n-1} - 2/3 \cdot (-1)^n \cdot 2^{2(n-1)}$ and the value changes with N as $2 + 5 \cdot N$). The coefficients in other terms rise not faster. Thus the coefficients arising by consecutive powers of hamiltonian rise not so quickly as $N!$ existing in the denominator of the evolution operator expansion terms. Thus skipped powers of (7) quickly disappear.

ACKNOWLEDGMENTS

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