# How long does it take (para-Ps AND ortho-Ps) to become (para-Ps OR ortho-Ps)?

# Decoherence of Positronium in Matter.

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# Positron applications



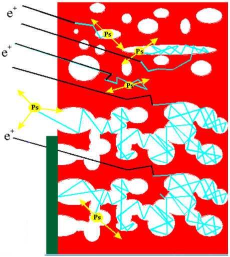
Positron techniques: PALS, ACAR, Doppler Broad. Spec.

Non-destructive nano-probe for:

- free volume (e.g., pores) size,

- study of the electron structure of the bulk

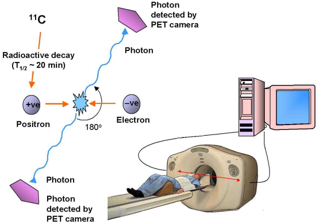
and of defects




resources:
http://positron.physik.uni-halle.de

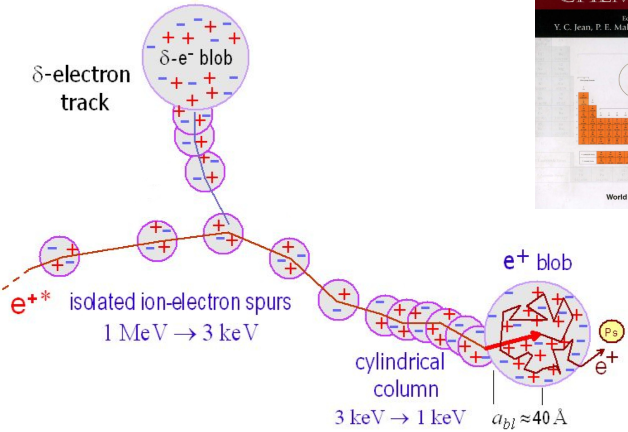
https://i.pinimg.com

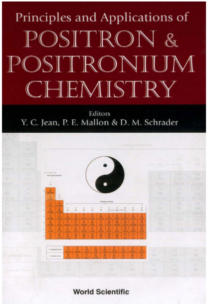
## Positron Emission Tomography



# The *blob* model





# para-, ortho- , 2-$\gamma$, 3-$\gamma$



## p-Ps, o-Ps

$$
\begin{aligned}
|S, m=0\rangle &= \frac{1}{\sqrt{2}}(|\uparrow\rangle_-|\downarrow\rangle_+ - |\downarrow\rangle_-|\uparrow\rangle_+) \\
|T, m=-1\rangle &= |\downarrow\rangle_-|\downarrow\rangle_+ \\
|T, m=0\rangle &= \frac{1}{\sqrt{2}}(|\uparrow\rangle_-|\downarrow\rangle_+ + |\downarrow\rangle_-|\uparrow\rangle_+) \\
|T, m=+1\rangle &= |\uparrow\rangle_-|\uparrow\rangle_+
\end{aligned}
$$

$$
\begin{aligned}
para-Ps: &\quad |S=0, m_S=0\rangle \longrightarrow 2\gamma \\
ortho-Ps: &\quad |S=1, m_S=-1,0,1\rangle \longrightarrow 3\gamma
\end{aligned}
$$

$\gamma \longrightarrow$ lifetime spectra

# $2\gamma$ from Ps in matter



- pick-off annihilation (with $e^-$ from an orbital)
- chemical quenching (due to chemical bond of Ps)
- ortho-para spin conversion (spin-orbit interaction)
- ortho-para spin conversion (electron exchange; paramagnetic molecules)

## QED states are PC – invariant

$$\pi_{PC} = -(-1)^S$$

| $^{2S+1}L_J$ | J | $\pi_P$ | $\pi_C$ | $\pi_{PC}$ |
|---|---|---|---|---|
| $^1S_0$ | 0 | -1 | +1 | -1 |
| $^1P_1$ | 1 | +1 | -1 | -1 |
| $^1D_2$ | 2 | -1 | +1 | -1 |

p-Ps

| $^{2S+1}L_J$ | J | $\pi_P$ | $\pi_C$ | $\pi_{PC}$ |
|---|---|---|---|---|
| $^3P_0$ | 0 | +1 | +1 | +1 |
| $^3S_1 + {}^3D_1$ | 1 | -1 | -1 | +1 |
| $^3P_1$ | 1 | +1 | +1 | +1 |

o-Ps

## C-parity invariance leads to a selection rule for decay

$$Ps: \quad \pi_C = (-1)^{L+S}$$

$$\gamma: \quad \pi_C = (-1)^n$$

# Motivation



Some facts:

- Energy difference between p-Ps and o-Ps is $8.4 \cdot 10^{-4}$ eV ($kT \simeq 2.5 \cdot 10^{-2}$eV).
- What if an electromagnetic interaction of the $e^{+} - e^{-}$ pair with other electrons does not prefer p-Ps, o-Ps basis? Its coupling constant is comparable to this for $e^{+} - e^{-}$ internal interaction.

Let us assume – Ps can exist in the cohered state of spins.
As long as Ps is in a superposition the number of photons per decay is not well defined.

# Motivation



M. Pietrow [1], P. Słomski

- spin conversion of valence electrons is possible for unpaired $e^-$ (paramagnetic mol., radicals, quasi-free $e^-$ who are present in the $e^+$ blob).
- spin interaction of a valence $e^-$ at a free volume wall may interfere with the Pauli principle.
- Ps bounces to the wall time to time only.

Interactions of $e^+ - e^-$ with environmental electrons (spin bath), via a spin space, can change the spin of the pair.
Does it lead to the p-Ps and o-Ps?
How long does it take?

# Decoherence (general). Schrödinger cat problem.



M. Pietrow [1], P. Słomski

Q. decoherence plays an important role in explanation of Schrödinger cat states reduction.

It is a process of coupling the system with environmental modes which leads to erase off-diagonal terms in the reduced density matrix of the system.

Here, it allows for decaying the Ps state from a superposition state.

# Decoherence (general). Schrödinger cat problem.

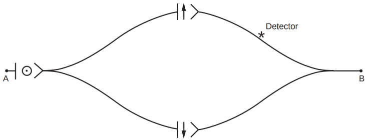


**initial state**

$\Phi^{(i)} = |\psi_{\mathcal{S}}\rangle\, |d_{\downarrow}\rangle$,
where $|\psi_{\mathcal{S}}\rangle = \alpha|\uparrow\rangle + \beta|\downarrow\rangle$

**final state**

$\Phi^{(f)} = \alpha|\uparrow\rangle|d_{\uparrow}\rangle + \beta|\downarrow\rangle|d_{\downarrow}\rangle$




W.H. Żurek: Physics Today, 44:36-44 (1991)

## Schrödinger cat probel:

Does it mean that the system is described by alternatives before asking the detector?

Or does it mean simply description of the ignorance of the observer about the outcome and does not describe a real final state? What the state evolves in time?

# Decoherence. Non-unitary reduction of the state



M. Pietrow [1], P. Słomski

$$\rho^{(f)} \xrightarrow[\text{decoherence},\, H_{int}]{} \rho^{(r)}$$

coherent system

$$\begin{aligned}
\rho^{(f)} &= |\Phi^{(f)}\rangle\langle\Phi^{(f)}| = \\
&= |\alpha|^2 \cdot |\uparrow\rangle\langle\uparrow| \cdot |d_\uparrow\rangle\langle d_\uparrow| + |\beta|^2 \cdot |\downarrow\rangle\langle\downarrow| \cdot |d_\downarrow\rangle\langle d_\downarrow| + \\
&+ \alpha\beta^* \cdot |\uparrow\rangle\langle\downarrow| \cdot |d_\uparrow\rangle\langle d_\downarrow| + \alpha^*\beta \cdot |\downarrow\rangle\langle\uparrow| \cdot |d_\downarrow\rangle\langle d_\uparrow|
\end{aligned}$$

# Decoherence. Non-unitary reduction of the state



$$\rho^{(f)} \xrightarrow[\text{decoherence},\ H_{int}]{} \rho^{(r)}$$

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&+ \alpha\beta^* \cdot |\uparrow\rangle\langle\downarrow| \cdot |d_\uparrow\rangle\langle d_\downarrow| + \alpha^*\beta \cdot |\downarrow\rangle\langle\uparrow| \cdot |d_\downarrow\rangle\langle d_\uparrow|
\end{aligned}$$

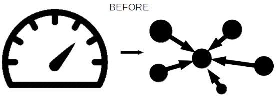
goes to a reduced one

$$\begin{aligned}
\rho^{(r)} &= |\Phi^{(f)}\rangle\langle\Phi^{(f)}| = \\
&= |\alpha|^2 \cdot |\uparrow\rangle\langle\uparrow| \cdot |d_\uparrow\rangle\langle d_\uparrow| + |\beta|^2 \cdot |\downarrow\rangle\langle\downarrow| \cdot |d_\downarrow\rangle\langle d_\downarrow| + \\
&+ \cancel{\alpha\beta^* \cdot |\uparrow\rangle\langle\downarrow| \cdot |d_\uparrow\rangle\langle d_\downarrow|} + \cancel{\alpha^*\beta \cdot |\downarrow\rangle\langle\uparrow| \cdot |d_\downarrow\rangle\langle d_\uparrow|}
\end{aligned}$$

# Decoherence (general). Interaction and reading

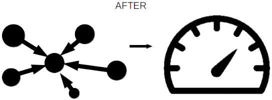


## Measurement BEFORE interaction with environment




$$\rho^{(B)} = |\psi\rangle\,|\epsilon\rangle\langle\epsilon|\langle\psi| = $$
$$= \sum_i \alpha_i|\psi_i\rangle \sum_j \beta_j|\epsilon_j\rangle \sum_k \beta_k^*\langle\epsilon_k| \sum_l \alpha_l^*\langle\psi_l|$$

## Measurement AFTER interaction with environment




$$\rho^{(A)} = \sum_i |\psi_i\rangle\,|\epsilon_i\rangle \sum_j \langle\epsilon_j|\langle\psi_j|$$

# Decoherence (general). Interaction and reading



Reduced density matrix:
BEFORE interaction with environment

$$\rho_{red}^{(B)} = Tr_{env}(\rho) = \sum_i \langle\epsilon_i| \left(|\psi|\epsilon\rangle\langle\epsilon|\langle\psi|\right) |\epsilon_i\rangle = \cdots$$
$$= \cdots = \sum_{i,j} \alpha_i \alpha_j^* |\psi_i\rangle\langle\psi_j|$$

and AFTER that

$$\rho_{red}^{(A)} = Tr_{env}(\rho) = \sum_k \langle\epsilon_k|\ \rho\ |\epsilon_k\rangle =$$
$$= \cdots = \sum_k |\alpha_k|^2\ |\psi_k\rangle\langle\psi_k|$$

# Decoherence (general). Interaction and reading



M. Pietrow [1], P. Słomski

Transition probability $\psi \longrightarrow \phi$:
BEFORE

$$\begin{aligned} \langle\phi|\rho_{red}^{(B)}|\phi\rangle &= \sum_{i,j}\langle\phi_i^*|\rho_{red}|\phi_j\rangle = \\ &= \sum_i |\alpha_i|^2\ |\beta_i|^2 + \sum_{i\neq j}\alpha_i\alpha_j^*\beta_i^*\beta_j \end{aligned}$$

whereas AFTER

$$\begin{aligned} \langle\phi|\rho_{red}^{(A)}|\phi\rangle &= \sum_{i,j}\langle\phi_i^*|\rho_{red}|\phi_j\rangle = \\ &= \sum_i |\alpha_i|^2\ |\beta_i|^2 \end{aligned}$$

# Spin decoherence in the literature

How long does it take (para-Ps AND ortho-Ps) to become (para-Ps OR ortho-Ps)?

Decoherence of Positronium in Matter.

M. Pietrow [1], P. Słomski

VOLUME 90, NUMBER 21 PHYSICAL REVIEW LETTERS week ending 30 MAY 2003

## Quantum Oscillations without Quantum Coherence

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(Received 8 December 2001; published 30 May 2003)

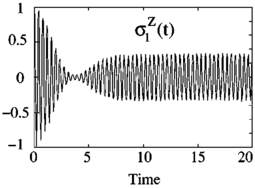
We study numerically the damping of quantum oscillations and the dynamics of the density matrix in model many-spin systems decohered by a spin bath. We show that oscillations of some density matrix elements can persist with considerable amplitude long after other elements, along with the entropy, have come close to saturation, i.e., when the system has been decohered almost completely. The oscillations exhibit very slow decay, and may be observable in experiments.

DOI: 10.1103/PhysRevLett.90.210401 PACS numbers: 03.65.Yz, 03.65.Ta, 75.10.Jm, 76.60.Es

For a quantum system prepared in a linear superposition of its eigenstates, some observables can oscillate with time. Interaction of the system with its environment leads to a decay of the system's initial pure state into a mixture of several states; i.e., nondiagonal elements of the density matrix vanish, and diagonal elements achieve

strate very slow damping, which is not related to thermalization of the system. The existence of rapid quantum oscillations in a decohered system is in striking contrast with the standard scenario of decoherence, and, to our knowledge, has not been discussed before.

We consider a system weakly coupled to the environ-




PHYSICAL REVIEW B **70**, 014435 (2004)

## Parity effects in spin decoherence

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(Received 11 February 2004; revised manuscript received 14 April 2004; published 30 July 2004)

We demonstrate that decoherence of many-spin systems can drastically differ from decoherence of single-spin systems. The difference originates at the most basic level, being determined by parity of the central system, i.e., by whether the system comprises even or odd number of spin-1/2 entities. Therefore, it is very likely that similar distinction between the central spin systems of even and odd parity is important in many other situations. Our consideration clarifies the physical origin of the unusual two-step decoherence found previously in the two-spin systems.

DOI: 10.1103/PhysRevB.70.014435 PACS number(s): 75.10.Jm, 03.65.Yz, 76.60.Es, 03.65.Ta

### I. INTRODUCTION

Reduced dynamics of a small quantum system coupled to

originates at the most basic level, and is determined primarily by parity of a central system, i.e., by whether the central

# Reference to our calculations



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## The role of positronium decoherence in positron annihilation in matter

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ABSTRACT

A small difference between the energies of the para-positronium (p-Ps) and ortho-positronium (o-Ps) states suggests the possibility of the superposition of p-Ps and o-Ps during the formation of positronium (Ps) from pre-Ps, terminating its migration in the matter in a void. It is shown that such a superposition decoheres in the basis of p-Ps and o-Ps. The decoherence time scale estimated here motivates a correction in the precise analysis of the positron annihilation lifetime spectra. More generally, the superposited Ps state should contribute to the theory of the evolution of positronium in matter.



**1. Introduction**

The most powerful model describing the formation of the positronium atom in matter was developed by Stepanov and Byakov [1]. A positron from a radioactive source passing through a sample creates products including electrons, ions, and radicals, losing its own energy in the process. The positron comes to rest

Positron annihilation is widely used in studies of the properties of matter, such as the free volume distribution [2], and of the trapping electrons produced during irradiation processes [3]. One of the most common positronic measurement techniques is Positron Annihilation Lifetime Spectroscopy (PALS) [4], which measures the time between the creation and annihilation of a positron (and its bound state, positronium). The lifetime of each positron fraction is related in some way to the properties of the sample where the an-

# Decoherence for $e^+ - e^-$



M. Pietrow [1], P. Słomski

Let assume permanent interaction of $e^+ - e^-$ with $N$ electron spins

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

$\rho_0 \equiv |\Psi_0\rangle\langle\Psi_0|$, where

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

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

# Decoherence for $e^+ - e^-$



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

where $|\Psi_t\rangle = e^{-iHt/\hbar}|\Psi_0\rangle$.

Time evolution is given by

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

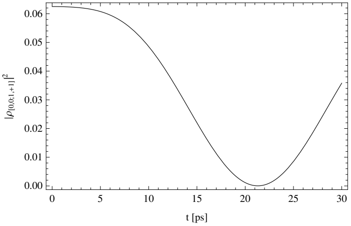
$$|\Psi_t\rangle = e^{-iHt/\hbar}|\Psi_0\rangle \simeq \sum_{j=0}^{n} \frac{1}{j!}(-\frac{itH}{\hbar})^j \; |\Psi_0\rangle, \tag{6}$$

# Results



## The measure of nondiagonality

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




$|\rho_{[0,0;1,+1]}(t)|^2$

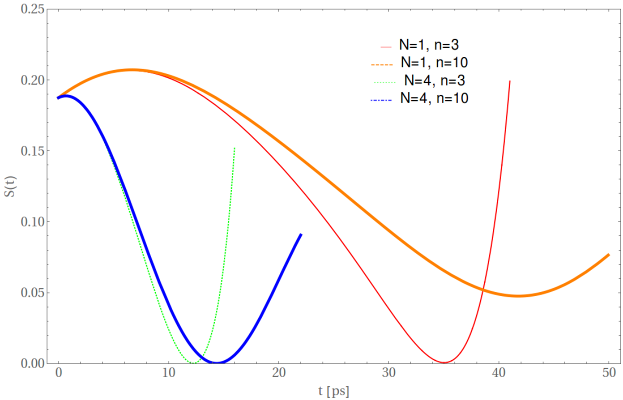
$N$=2 (random init.), $n$=10.

# Results- decoherence may last tenths of ps

How long does it take (para-Ps AND ortho-Ps) to become (para-Ps OR ortho-Ps)?

Decoherence of Positronium in Matter.

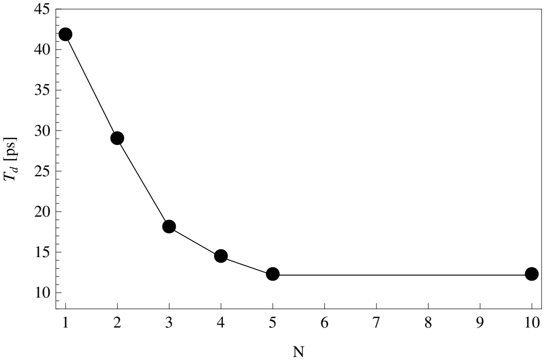
M. Pietrow [1], P. Słomski




$S(t)$ averaged over 100 rand. $|S\rangle$.

# Results. $T_d$ decreases with $N$






Averaged over 20 randomly chosen initial state vectors.

$n$=7

! asymptotic $T_d$ value is visible

# $J$ coupling constant

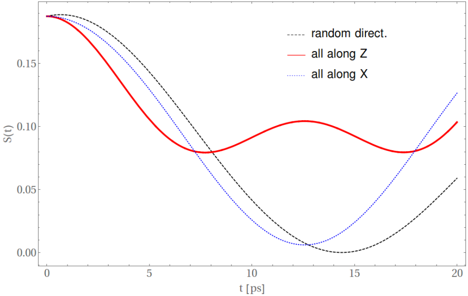


M. Pietrow [1], P. Słomski

Here, $J\frac{\hbar^2}{4}$ in $H_{int}$ is set as $10^{-4}$ eV (ortho-para conversion energy).
However, for $N = 3$:
if $J\frac{\hbar^2}{4}$=$10^{-5}$ eV $\Longrightarrow$ $T_d \simeq 150$ ps
instead of $T_d \simeq 18$ ps estimated for $J\frac{\hbar^2}{4}$=$10^{-4}$ eV.

In larger free volumes ($2R \gg \lambda$=3.6 nm) a pair interacts with the wall only from time to time $\Longrightarrow J = J(t)$.

# Results. Magnetization of the medium



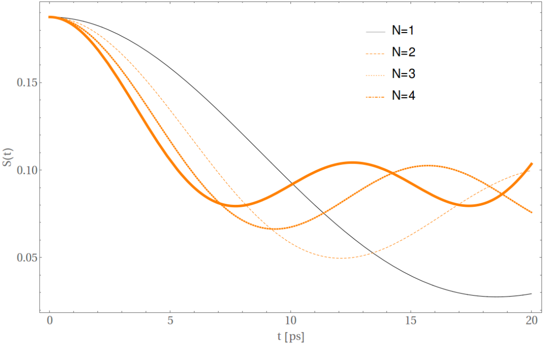

$N$=4, $n$=10, av. over 100

Warning 1: $H$ Eigenstates of Ps in magnetic field are superposition of p-Ps and o-Ps.
Warning 2: It is known that Ps does not form in ferromagnetic crystals.

# Results. Magnetization along the $z$-axis




M. Pietrow [1], P. Słomski

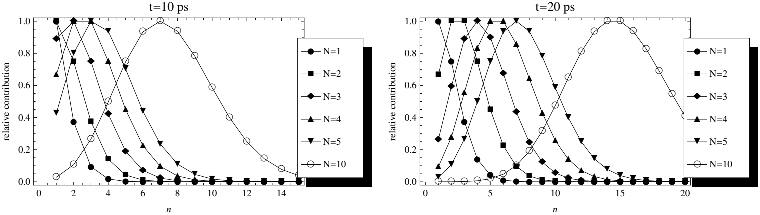
# Results. Relative account of terms. Slowly covergent expression.



Next terms

$$H^n = \left(\sum_{p=3}^{N+2} \sigma^{(2)} \circ \sigma^{(p)}\right)^n = \sum_{p,s,t,\ldots}^{n\text{-fold sum}} \sigma^{(2)} \circ \sigma^{(p)} \cdot \sigma^{(2)} \circ \sigma^{(s)} \cdot \ldots$$

in interaction Hamiltonian expansion may not be to neglect.




E.g., for $N$=10, a greatest contribution gives $n$=$7^{th}$ term of $H_{int}$ expansion at $t$=10 ps.

# Decay rate of positrons. Link to PALS spectra.

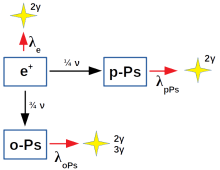
How long does it take (para-Ps AND ortho-Ps) to become (para-Ps OR ortho-Ps)?

Decoherence of Positronium in Matter.

M. Pietrow [1], P. Słomski

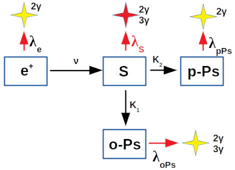
Now, the dynamics of positron population is estimated by

$$\begin{cases} dP_e(t) = -(\lambda_e + \nu) P_e(t) dt, & P_e(0) = 1, \\ d(oPs)(t) = \frac{3}{4} \nu P_e(t) dt - \lambda_{oPs} (oPs)(t) dt, & (oPs)(0) = 0, \\ d(pPs)(t) = \frac{1}{4} \nu P_e(t) dt - \lambda_{pPs} (pPs)(t) dt, & (pPs)(0) = 0 \end{cases}$$




the decoherence causes its modification

$$\begin{cases} dP_e(t) = -(\lambda_e + \nu) P_e(t) dt, & P_e(0) = 1, \\ dS(t) = \nu P_e(t) dt - (\lambda_S + K) S(t) dt, & S(0) = 0, \\ d(oPs)(t) = K_1 \, S(t) dt - \lambda_{oPs} (oPs)(t) dt, & (oPs)(0) = 0, \\ d(pPs)(t) = K_2 \, S(t) dt - \lambda_{pPs} (pPs)(t) dt, & (pPs)(0) = 0 \end{cases}$$




where $K_1 + K_2 = K$.

# $\gamma$ spectra for PALS



Now in PALS, the gamma spectra are decomposed into

$$dN_\gamma \sim -dP_e^{(\lambda_e)} - d(pPs)^{(\lambda_{pPs})} - d(oPs)^{(\lambda_{oPs})}$$

The influence of the decoherence causes its modification

$$dN_\gamma \sim -dP_e^{(\lambda_e)} - dS^{(\lambda_S)} - d(pPs)^{(\lambda_{pPs})} - d(oPs)^{(\lambda_{oPs})}.$$

Most of the annihilation is $2\gamma$ in matter. The additional element in the equation is responsible for an increase of $3\gamma$ annihilation as long as the cohered state exists.

# Summary 1/2



- Indeed, $S(t)$ decreases. Ps(t) (almost) decoheres in basis of the p-Ps and o-Ps. After $S(t)$ collapsing oscillations appear.
- The calculated timescale of $T_d$ is pico-secs. Thus, the process of spin decoherence may affect the gamma spectra for short living positrons.
- $T_d$ decreases with the number of electrons $N$ in the bath.
- $T_d$ depends strongly on the value of coupling constant $J$.

# Summary 2/2



M. Pietrow [1], P. Słomski

- Higher orders of the Hamiltonian in the evolution operator give important contribution to calculated $T_d$ but do not change the timescale of it.
- Magnetization of the medium speeds up the decoherence and suppresses the effectiveness of it.
- More realistic interaction Hamiltonians are needed. In particular, $J = J(t)$ need to be considered.