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1998 J. Phys.: Condens. Matter 10 10461

(http://iopscience.iop.org/0953-8984/10/46/014)

J. Phys.: Condens. Matter **10** (1998) 10461–10474. Printed in the UK PII: S0953-8984(98)97373-8

An analytical theory of the slowing down and the thermalization of positrons in condensed matter

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Received 30 April 1998

Abstract. The paper outlines an analytical treatment of the slowing down of positrons (e^+) implanted into condensed matter based on the rather weak assumption that the loss of energy or momentum and the scattering angle are uniquely related. It goes beyond the mathematical techniques developed for the slowing down of neutrons by allowing for the annihilation rate of positrons and making use of the fact that for e^+, owing to its small mass, the energy loss per collision is usually very small compared with the kinetic energy. Explicit expressions are given for the sample-averaged momentum distribution of positrons as a function of the positron age and for the distribution function in space, momentum magnitude, and time of positronium that is slowed down by the interaction with optical phonons.

1. Introduction

During the past four decades, the annihilation of positrons (e^+) has become an indispensable tool in condensed matter studies. The interpretation of the information contained in the annihilation radiation is very often based on the assumption that the positrons are thermalized in times that are short compared with the positron lifetime, so that annihilation 'in flight' (in contrast to annihilation while the e^+ are diffusing in thermal equilibrium with their environment or are trapped at, say, crystal imperfections) may be neglected. The time interval between the implantation of an e^+ into condensed matter until its kinetic energy has been reduced to $3k_BT/2$ (k_B = Boltzmann's constant, T = absolute temperature) may be subdivided into a slowing-down period and a thermalization period according to the following criterion. In the slowing period the rate of loss of the e^+ energy is temperature independent, whereas the loss mechanisms dominating during the thermalization period (usually involving phonons) depend on the sample temperature T.

Typical kinetic energies with which e^+ originating from the β^+-decay of a neutron-deficient nuclide without moderation or acceleration are implanted into condensed matter are in the range 0.1 MeV to a few MeV. Positrons in so-called slow-positron beams have typically kinetic energies between a few keV and about 50 keV (a more descriptive name is therefore 'keV beams'). In these two modes of implantation the in-flight annihilation may usually be neglected. This is not so for MeV beams (also called 'relativistic' e^+ beams), an example of which (the Stuttgart beam [1]) usually operates at an e^+ kinetic energy of 4 MeV. Lauff [2] has estimated that in this case about 0.15 of the positrons implanted into Pb annihilate in flight.

For the most important loss mechanisms the energy-loss rate, $-\mathrm{d}E/\mathrm{d}t$, is known; so for a given starting energy of the e^+ the slowing-down and thermalization periods may be estimated. The situation is quite different with regard to the spatial distribution of the implanted positrons. Since the mass of the positrons is small compared to the atomic masses, scattering through large angles is rather frequent. This has the well-known consequence that already during the slowing-down period the e^+ motion becomes diffusive and that, therefore, the e^+ do not have a characteristic range, in contrast to heavier electrically charged particles such as protons, deuterons, or α-particles. For many applications, in particular for the use of keV beams of adjustable energy to study depth profiles of trapping sites in layered materials, it is of utmost importance to be able to calculate the spatial distribution of the implanted e^+.

A related problem of some practical interest is the following: when e^+ capture an electron (e^-) to form positronium, $\mathrm{Ps} = (e^+e^-)$, the energy-loss rate is suddenly reduced since owing to the electrical neutrality of Ps the mechanisms primarily responsible for the slowing down of the e^+ cease to operate [3]. What are the chances for the neutral Ps 'atoms' to escape from the 'spur' of electrons and defect electrons (holes) that the e^+ had produced before Ps was formed? To answer this question we must be able to estimate, as a function of time t and distance $\boldsymbol{r}$, the probability distribution of Ps generated at $t = 0$ and $\boldsymbol{r} = 0$.

So far, the types of question sketched in the preceding paragraphs have been approached preferentially by Monte Carlo computer simulations since, except for a few very simplified cases, the situations appeared too complicated to be handled analytically. This view appears to have overlooked the fact that very similar problems arose about six decades ago in investigations of the slowing down of neutrons in cosmic-ray studies [4–7] and not much later in the design of nuclear reactors [8–13]. It is the aim of the present paper to adopt and, where necessary, to supplement the earlier work on the slowing down of neutrons for the positron and positronium case. It will be shown that it is possible to proceed quite a long way by analytical techniques and that the numerical work can be postponed till the very last stage of the calculations, when specific slowing-down and thermalization mechanisms have to be taken into account. Moreover, the computations that may eventually be required are quite straightforward once the mechanisms of energy loss and scattering are known.

The present paper gives a brief outline of the theory and of the underlying physical ideas and mathematical techniques. A more detailed account was submitted to SLOPOS (the Symposium on Slow Positron Beams, held in Cape Town in September 1998, to be published in *Applied Surface Science*). As an example we treat the slowing down of light particles due to their interaction with phonons describable by the Einstein model (so-called optical phonons). This is thought to be a good model for the slowing down of positronium in all positronium-forming substances with optical phonon branches (i.e., in all condensed Ps-formers with the exception of the rare gases) [3].

2. The transport equation

In the following the particles (e^+ or Ps) are described as an ensemble that is dilute enough for any interaction between them to be neglected. The independent variables are the location $\boldsymbol{r}$, the momentum $p\boldsymbol{\Omega}$, where $\boldsymbol{\Omega}$ is a unit vector (in the following frequently referred to as the 'flight direction'), and the time t. We will have to consider four different distribution functions. The simplest of them are the *differential number density* $n(\boldsymbol{r}, \boldsymbol{\Omega}, p; t)$ and the *differential particle flux* $\boldsymbol{\Phi}(\boldsymbol{r}, \boldsymbol{\Omega}, p; t)$. The quantity $n(\boldsymbol{r}, \boldsymbol{\Omega}, p; t)\ \mathrm{d}^3\boldsymbol{r}\ \mathrm{d}^2\boldsymbol{\Omega}\ \mathrm{d}p$ is the number of particles in the six-dimensional 'volume element' $\mathrm{d}^3\boldsymbol{r}\ \mathrm{d}^2\boldsymbol{\Omega}\ \mathrm{d}p$ (or, with suitable normalization, the probability of finding a particle in this volume element) at time

t. Number density and particle flux are related by

$$\boldsymbol{\Phi}(\boldsymbol{r}, \boldsymbol{\Omega}, p; t) = v n(\boldsymbol{r}, \boldsymbol{\Omega}, p; t), \tag{1}$$

where v is the velocity of the particles. Often we are not interested in the dependence on all of the independent variables in (1). If we integrate over $\boldsymbol{\Omega}$ or p, we simply drop these quantities in the arguments. For example, the *particle density* is

$$n(\boldsymbol{r}, t) = \oint \int_0^\infty n(\boldsymbol{r}, \boldsymbol{\Omega}, p; t)\ \mathrm{d}p\ \mathrm{d}^2\boldsymbol{\Omega} \tag{2}$$

($\oint$ signifies that the $\boldsymbol{\Omega}$-integration extends over the full solid angle, 4π sr) and the particle flux is

$$\boldsymbol{\Phi}(\boldsymbol{r}, t) = \oint \int_0^\infty v(p) n(\boldsymbol{r}, \boldsymbol{\Omega}, p; t)\ \mathrm{d}p\ \mathrm{d}^2\boldsymbol{\Omega} =: \langle v \rangle n(\boldsymbol{r}, t), \tag{3}$$

where the right-hand equation [3] defines the average speed $\langle v \rangle$. The two other distribution functions required, the event-rate density $\boldsymbol{\Psi}$ and the slowing-down density $\boldsymbol{\Xi}$, will be defined later.

Depending on the choice of the dependent variables and of the spatial coordinate system, the transport equation, which expresses the local balance of the differential number density, may be written in different forms. If we multiply the first form,

$$\begin{aligned}\frac{\partial n(\boldsymbol{r}, \boldsymbol{\Omega}, p; t)}{\partial t} &= -\boldsymbol{\Omega} \cdot \operatorname{grad} \boldsymbol{\Phi}(\boldsymbol{r}, \boldsymbol{\Omega}, p; t) - (\boldsymbol{\Sigma}_\mathrm{s} + \boldsymbol{\Sigma}_\mathrm{a}) \boldsymbol{\Phi}(\boldsymbol{r}, \boldsymbol{\Omega}, p; t) \\ &\quad + \int_0^\infty \oint \boldsymbol{\Sigma}_\mathrm{s}(\boldsymbol{\Omega}' \to \boldsymbol{\Omega}, p' \to p) \boldsymbol{\Phi}(\boldsymbol{r}, \boldsymbol{\Omega}', p; t)\ \mathrm{d}^2\boldsymbol{\Omega}'\ \mathrm{d}p' + S(\boldsymbol{r}, \boldsymbol{\Omega}, p; t),\end{aligned} \tag{4}$$

with the six-dimensional volume element $\mathrm{d}^3\boldsymbol{r}\ \mathrm{d}^2\boldsymbol{\Omega}\ \mathrm{d}p$, the left-hand side becomes the *rate of change* of the number of particles in that volume element. The first term on the right-hand side is then the differential *rate of leakage* out of $\mathrm{d}^3\boldsymbol{r}$, the second one the sum of the *losses by scattering* into other flight directions and by *annihilation and trapping* of e^+ or Ps. This term describes the loss by scattering in terms of the *macroscopic scattering cross section* $\boldsymbol{\Sigma}_\mathrm{s} = \boldsymbol{\Sigma}_\mathrm{s}(p)$, which is equal to the inverse of the mean free path between scattering events, l_s^{-1}. The macroscopic cross section $\boldsymbol{\Sigma}_\mathrm{a}$ accounts for both *annihilation* and *trapping*. For non-relativistic positrons the annihilation rate and hence their mean lifetime, $\overline{\tau}$, are velocity independent. Thus the contribution of *annihilation* to the macroscopic cross section $\boldsymbol{\Sigma}_\mathrm{a}$ may be written as

$$\boldsymbol{\Sigma}_\mathrm{a}(p) = (\overline{\tau} v)^{-1} =: l_\mathrm{a}^{-1}, \tag{5}$$

where l_a is the 'mean free path for annihilation'. The *trapping rate* may show resonances as a function of p; well below such resonances its contribution to $\boldsymbol{\Sigma}_\mathrm{a}$ has the velocity dependence (5), too.

The third term on the right-hand side of (4) accounts for the *gain* by in-scattering into $\mathrm{d}^3\boldsymbol{r}\ \mathrm{d}^2\boldsymbol{\Omega}\ \mathrm{d}p$ from flight directions other than $\boldsymbol{\Omega}$ and momentum magnitudes other than p. The relationship between the scattering cross sections appearing in the second and third term on the right-hand side of (4) is

$$\boldsymbol{\Sigma}_\mathrm{s}(p) = \int_0^\infty \boldsymbol{\Sigma}_\mathrm{s}(p' \to p)\ \mathrm{d}p' \tag{6}$$

with

$$\boldsymbol{\Sigma}_\mathrm{s}(p' \to p) := \oint \boldsymbol{\Sigma}_\mathrm{s}(\boldsymbol{\Omega}' \to \boldsymbol{\Omega}, p' \to p)\ \mathrm{d}^2\boldsymbol{\Omega}'. \tag{7}$$

Finally, the last term in (4) describes internal sources of e^+ or Ps. In many cases it may be replaced by suitable initial and boundary conditions, so that the equation to be solved becomes homogeneous. In the discussion of the mathematical techniques we shall therefore emphasize solving the homogeneous transport equation.

The transport equation (4) may be given another form by introducing the *differential event rate density*

$$\boldsymbol{\Psi}(\boldsymbol{r},\boldsymbol{\Omega},p;t) := \left[\boldsymbol{\Sigma}_{\mathrm{s}}(p)+\boldsymbol{\Sigma}_{\mathrm{a}}(p)\right]\boldsymbol{\Phi}(\boldsymbol{r},\boldsymbol{\Omega},p;t) \tag{8}$$

as the dependent variable. For homogeneous media (i.e., macroscopic cross sections that are $\boldsymbol{r}$-independent) this leads to

$$\begin{aligned}\frac{1}{(\boldsymbol{\Sigma}_{\mathrm{a}}+\boldsymbol{\Sigma}_{\mathrm{a}})v}\frac{\partial\boldsymbol{\Psi}(\boldsymbol{r},\boldsymbol{\Omega},p;t)}{\partial t}&+\frac{1}{\boldsymbol{\Sigma}_{\mathrm{s}}+\boldsymbol{\Sigma}_{\mathrm{a}}}\boldsymbol{\Omega}\cdot\mathrm{grad}\,\boldsymbol{\Psi}(\boldsymbol{r},\boldsymbol{\Omega},p;t)+\boldsymbol{\Psi}(\boldsymbol{r},\boldsymbol{\Omega},p;t)\\ &=\int\frac{\boldsymbol{\Sigma}_{\mathrm{s}}(p')}{\boldsymbol{\Sigma}_{\mathrm{s}}(p')+\boldsymbol{\Sigma}_{\mathrm{a}}(p')}\oint\frac{\boldsymbol{\Sigma}_{\mathrm{s}}(\boldsymbol{\Omega}'\to\boldsymbol{\Omega},p'\to p)}{\boldsymbol{\Sigma}_{\mathrm{s}}}\boldsymbol{\Psi}(\boldsymbol{r},\boldsymbol{\Omega}',p';t)\,\mathrm{d}\boldsymbol{\Omega}'\,\mathrm{d}p'\\ &\quad+S(\boldsymbol{r},\boldsymbol{\Omega},p;t).\end{aligned} \tag{9}$$

In transport problems the direction of the net flow of particles provides us with a preferred space direction, which we may use as the z-axis of a polar coordinate system. If the direction cosine with respect to this direction is denoted by $\cos\vartheta$, the homogeneous equation (9) may be written as

$$\begin{aligned}\frac{1}{\boldsymbol{\Sigma}_{\mathrm{s}}(p)+\boldsymbol{\Sigma}_{\mathrm{a}}(p)}&\left[\frac{1}{v}\frac{\partial\boldsymbol{\Psi}(\boldsymbol{r},\boldsymbol{\Omega},p;t)}{\partial t}+\cos\vartheta\frac{\partial\boldsymbol{\Psi}(\boldsymbol{r},\boldsymbol{\Omega},p;t)}{\partial z}\right]+\boldsymbol{\Psi}(\boldsymbol{r},\boldsymbol{\Omega},p;t)\\ &=\int_0^\infty\frac{\boldsymbol{\Sigma}_{\mathrm{s}}(p')}{\boldsymbol{\Sigma}_{\mathrm{s}}(p')+\boldsymbol{\Sigma}_{\mathrm{a}}(p')}\oint\frac{\boldsymbol{\Sigma}_{\mathrm{s}}(\boldsymbol{\Omega}'\to\boldsymbol{\Omega},p'\to p)}{\boldsymbol{\Sigma}_{\mathrm{s}}(p')}\boldsymbol{\Psi}(\boldsymbol{r},\boldsymbol{\Omega}',p';t)\,\mathrm{d}^2\boldsymbol{\Omega}'\,\mathrm{d}p'.\end{aligned} \tag{10}$$

Equation (10) is a form of the transport equation that is frequently used in astrophysics. [14, 15]. It shows that for plane problems, in which there is only one relevant spatial coordinate, solutions may be factorized with spatial factors $\exp(\pm\kappa z)$, where κ is an eigenvalue parameter [13]. We shall return to (10) in section 6.

Equations (4), (9), (10) are linear integro-differential equations that allow us, in principle, to calculate n, $\boldsymbol{\Phi}$, or $\boldsymbol{\Psi}$ for a given scattering mechanism and for given initial and boundary conditions. They are, however, too complicated to be solved exactly in non-trivial cases. Our next task is to simply the equations in ways that allow us to obtain good approximate solutions for specific problems. Important steps are the introduction of the momentum scattering probability, $g_p(p'\to p)$, and of the fourth dependent variable, the slowing-down density $\boldsymbol{\Xi}(\boldsymbol{r},p;t)$.

3. Momentum scattering probability and slowing-down density

The *momentum scattering probability*

$$g_p(p'\to p) := \frac{\boldsymbol{\Sigma}_{\mathrm{s}}(p'\to p)}{\boldsymbol{\Sigma}_{\mathrm{s}}(p)} \tag{11}$$

is defined as the probability that a scattering process changes the magnitude of the particle momentum from its initial value p' to a value in a unit interval around p. For the time being we confine ourselves to cases in which the target is at rest in the laboratory system (the system introduced at the beginning of section 2) and where internal degrees of freedom of the target do not come into play. (Such scattering events are usually called 'elastic', although the nomenclature is not uniform.) Since under these circumstances the energy and the momentum magnitude of scattered particles cannot increase, $g_p(p' \to p)$ is zero for $p > p'$. If $\beta p'$ denotes the lower limit of the momentum magnitude *after* the scattering event, $g_p(p' \to p)$ is different from zero only if p lies in the interval $[\beta p', p']$ with $0 \leqslant \beta < 1$, called the *collision interval*. The lower limit $\beta = 0$ is reached for two-body collisions of particles with equal masses. The fact that, owing to the small e^+ mass, for most positron scattering mechanisms β is very close to unity will play an important rôle in the following developments.

The probability that a particle with initial momentum magnitude $p' > p$ has a momentum magnitude $p'' < p$ after scattering is given by

$$G(p', p) = \int_{p''=\beta p'}^{p''=p} = g_p(p' \to p'')\, \mathrm{d}p. \tag{12}$$

Obvious properties of $G(p', p)$ are

$$\partial G(p', p)/\partial p = g_p(p' \to p), \tag{13a}$$

$$G(p/\beta, p) \equiv 0, \tag{13b}$$

$$G(p, p) \equiv 1. \tag{13c}$$

From (13*b*), (13*c*) it follows that as a function of the first of its independent variables, $G(p', p)$ *always* varies between 0 and 1, no matter how narrow the collision interval is.

An important quantity that may be expressed in terms of either $g_p(p' \to p)$ or $G(p', p)$ is the average *logarithmic* momentum loss per collision, ξ_p, defined as the loss per collision of the logarithm of the momentum of particles with a given initial momentum magnitude p. We thus have

$$\xi_p := \langle \ln(p/p_0) - \ln(p'/p_0)\rangle_{p'} = \langle \ln(p/p')\rangle_{p'} = \int_{p'=\beta p}^{p'=p} \ln(p/p') g_p(p \to p')\, \mathrm{d}p', \tag{14}$$

where p_0 is an arbitrary reference momentum. Integration by parts gives us

$$\xi_p = \int_{p'=\beta p}^{p'=p} \frac{1}{p'} G(p, p')\, \mathrm{d}p' = \int_{\ln p'=\ln p - \ln(1/\beta)}^{\ln p'=\ln p} G(p, p')\, \mathrm{d}\ln p'. \tag{15}$$

The *slowing-down density* $\Xi(\boldsymbol{r}, p; t)$ is defined as the number of particles per unit volume that are slowed down past the momentum p per unit time. From the density of the rate of scattering events with initial momentum magnitude p',

$$\boldsymbol{\Sigma}_{\mathrm{s}}(p')\boldsymbol{\Phi}(\boldsymbol{r}, p'; t) = \frac{\boldsymbol{\Sigma}_{\mathrm{s}}(p')}{\boldsymbol{\Sigma}_{\mathrm{s}}(p') + \boldsymbol{\Sigma}_{\mathrm{a}}(p')} \boldsymbol{\Psi}(\boldsymbol{r}, p'; t), \tag{16}$$

we obtain that of the events leading to the final momentum p by multiplying (16) by $G(p', p)$ and integrating over all initial momenta. The slowing-down density is thus given by

$$\Xi(\boldsymbol{r}, p; t) := \int_{p'=p}^{p'=p/\beta} \frac{\boldsymbol{\Sigma}_{\mathrm{s}}(p')}{\boldsymbol{\Sigma}_{\mathrm{s}}(p') + \boldsymbol{\Sigma}_{\mathrm{a}}(p')} G(p', p) \boldsymbol{\Psi}(\boldsymbol{r}, p'; t)\, \mathrm{d}p'. \tag{17}$$

Taking into account (13*a*), we deduce from (17)

$$\frac{\partial \Xi(\boldsymbol{r}, p; t)}{\partial p} = \int_{p'=p}^{p'=p/\beta} \frac{\boldsymbol{\Sigma}_{\mathrm{s}}(p')}{\boldsymbol{\Sigma}_{\mathrm{s}}(p') + \boldsymbol{\Sigma}_{\mathrm{a}}(p')} g_p(p' \to p) \boldsymbol{\Psi}(\boldsymbol{r}, p'; t)\, \mathrm{d}p' - \frac{\boldsymbol{\Sigma}_{\mathrm{s}}(p)}{\boldsymbol{\Sigma}_{\mathrm{s}}(p) + \boldsymbol{\Sigma}_{\mathrm{a}}(p)} \boldsymbol{\Psi}(p). \tag{18}$$

Since according to (7) and (11) the scattering probability may be written as

$$g_p(p' \to p) = \left(\oint \mathbf{\Sigma}_\mathrm{s}(\mathbf{\Omega}' \to \mathbf{\Omega}, p' \to p)\ \mathrm{d}^2\mathbf{\Omega}' \right) \Big/ \mathbf{\Sigma}_\mathrm{s}(p) \tag{19}$$

we may use (18) to rewrite the transport equations, after integrating over all directions of flight, as

$$\begin{aligned} \frac{\partial \mathbf{\Xi}(\boldsymbol{r}, p; t)}{\partial p} - \frac{1}{\mathbf{\Sigma}_\mathrm{s}(p) + \mathbf{\Sigma}_\mathrm{a}(p)} \left[\frac{1}{v} \frac{\partial \mathbf{\Psi}(\boldsymbol{r}, p; t)}{\partial t} + \mathbf{\Sigma}_\mathrm{a}(p) \mathbf{\Psi}(\boldsymbol{r}, p; t) \right] + S(\boldsymbol{r}, p; t) \\ = \frac{1}{\mathbf{\Sigma}_\mathrm{s}(p) + \mathbf{\Sigma}_\mathrm{a}(p)} \oint \mathbf{\Omega} \cdot \operatorname{grad} \mathbf{\Psi}(\boldsymbol{r}, \mathbf{\Omega}, p; t)\ \mathrm{d}^2\mathbf{\Omega}. \end{aligned} \tag{20}$$

The pair of equations (17), (20) constitute a fourth form of the transport equation. They are much simpler than (4), (9), or (10) since they no longer contain $\mathbf{\Omega}$ as an independent variable save for on the right-hand side of (20), where $\mathbf{\Omega}$ still appears as a variable of integration. It is the handling of this term that determines the various approaches to the solution of the transport equation to be discussed in the remainder of the paper.

4. Narrow collision intervals

So far, the treatment of the linear transport equation has been general. In the present section we make use, for the first time in the present paper, of the fact that for positrons the collision interval is narrow, i.e. that β is close to unity.

Since the independent variables of $G(p_1, p_2)$ must appear in dimensionless combination, for narrow collision intervals we may write

$$G(p_1, p_2) = G(\ln(p_1/p_2)). \tag{21}$$

Inserting (21) into (15) allows us to replace p_2 by p_1 as the variable of integration, giving us

$$\xi_p = \int_{p_1=p_2}^{p_1=p_2/\beta} \frac{1}{p_1} G(p_1, p_2)\ \mathrm{d}p_1 = \int_{\ln p_1 = \ln p_2)}^{\ln p_1 = \ln p_2 + \ln(1/\beta)} G(p_1, p_2)\ \mathrm{d}\ln p_1. \tag{22}$$

Since in the limit $\beta \to 1$, $G(p_1, p_2)$ is the only quantity in the integral of (17) that varies appreciably over the collision interval, we may use (22) to replace (17) by

$$\begin{aligned} \mathbf{\Xi}(\boldsymbol{r}, p; t) &= \frac{\mathbf{\Sigma}_\mathrm{s}(p) p \mathbf{\Psi}(\boldsymbol{r}, p; t)}{\mathbf{\Sigma}_\mathrm{s}(p) + \mathbf{\Sigma}_\mathrm{a}(p)} \int_{p'=p}^{p'=p/\beta} \frac{1}{p'} G(p', p)\ \mathrm{d}p' \\ &= \frac{\mathbf{\Sigma}_\mathrm{s}(p)}{\mathbf{\Sigma}_\mathrm{s}(p) + \mathbf{\Sigma}_\mathrm{a}(p)} p \xi_p \mathbf{\Psi}(\boldsymbol{r}, p; t). \end{aligned} \tag{23}$$

5. Sample-integrated quantities

One way of handling the bothersome right-hand side of (20) is to make use of the identity

$$\operatorname{div}[\mathbf{\Psi}(\boldsymbol{r}, \mathbf{\Omega}, p; t)\mathbf{\Omega}] \equiv \mathbf{\Omega} \cdot \operatorname{grad} \mathbf{\Psi}(\boldsymbol{r}, \mathbf{\Omega}, p; t) \tag{24}$$

to integrate (20) and (23) over the entire sample (assumed to be homogeneous), and to employ Gauss's integral theorem in order to transform the right-hand side of (20) into an integral extending over the sample surface. With the convention that dropping the space variables from the arguments of the field quantities indicates integration over the entire sample, equation (20) becomes

$$\frac{\partial \Xi(p,t)}{\partial p} - \frac{1}{\Sigma_s(p)+\Sigma_a(p)}\left[\frac{1}{v}\frac{\partial \Psi(p,t)}{\partial t} + \Sigma_a \Psi(p,t)\right] + S(p,t) = \frac{1}{\Sigma_s(p)+\Sigma_a(p)} \oint\int\int_{\text{surface}} \Psi(\boldsymbol{r}, \Omega, p; t)\Omega \cdot \mathrm{d}^2\boldsymbol{A}\ \mathrm{d}^2\Omega, \tag{25}$$

where $\mathrm{d}^2\boldsymbol{A}$ denotes the vectorial surface elements of the sample.

Equation (24) may be very useful in the interpretation of positron annihilation experiments that integrate over the entire sample. Suppose that the sample is large enough for the escape of e^+ to be negligible. Then the right-hand side of (25) is zero. Making use of the relationship (23) between $\Xi(p,t)$ and $\Psi(p,t)$ gives us an inhomogeneous linear first-order partial differential equation for $\Xi(p,t)$ that may be easily solved by the mathematical technique to be described below. If the source emits positrons with a wide momentum distribution (as a β^+-source does), then the integration of (25) must be followed by convoluting the result with the p-distribution of the source.

Another situation of practical importance that may be described by means of (25) is the following. Positrons are injected through part of the sample surface (e.g., a planar surface of a slab). There are no internal sources; the escape of e^+ from the sample is negligible. Then the right-hand side of (25) is a known function of p and t that may be absorbed into $S(p,t)$, and the mathematical problem is the same as in the preceding example.

If we Laplace transform (25) with respect to time and denote the Laplace-transformed quantities by a tilde, e.g.

$$\tilde{\Xi}(p;\eta) = \int_0^\infty \Xi(p,t)\exp(-\eta t)\ \mathrm{d}t, \tag{26}$$

we obtain the ordinary first-order differential equation

$$\frac{\partial \Xi(p;\eta)}{\partial p} - \frac{\Sigma_a(p) + (\eta/v)\tilde{\Xi}(p;\eta)}{p\xi_p(p)\Sigma_s(p)} + \tilde{S}(p;\eta) + n(p,0) = 0. \tag{27}$$

Its general solution is

$$\tilde{\Xi}(p;\eta) = \exp\left(\eta\int \frac{\mathrm{d}p}{pv\xi_p(p)\Sigma_s(p)} + \int \frac{\Sigma_a(p)\ \mathrm{d}p}{p\xi_p(p)\Sigma_s(p)}\right) \times \left\{C - \int\left[\tilde{S}(p;\eta) + n(p,0^+)\right]\exp\left(-\int \frac{\Sigma_a(p') + (\eta/v(p'))}{p'\xi_p(p')\Sigma_s(p')}\ \mathrm{d}p'\right)\mathrm{d}p\right\}, \tag{28}$$

where C is a constant of integration.

As an example, consider the creation of n_0 particles with a fixed momentum p_0 at time $t = 0$. This may be taken into account either through the source term $\tilde{S}(p,\eta)$ or through the initial condition $n(p,0) = n_0\delta(p - p_0)$. In either case these terms are proportional to a δ-function of $p_0 - p'$. This means that the p-integration inside the curly bracket of (28) may be carried out immediately, yielding a constant that may be absorbed in the constant of integration, C. We thus get for the Laplace transform of the sample-averaged slowing-down density

$$\tilde{\Xi}(p;\eta) = C\exp\left[-\int_{p'=p}^{p_0} \frac{\Sigma_a(p')\ \mathrm{d}p'}{p'\xi_p(p')\Sigma_s(p')}\ \mathrm{d}p'\right]\exp\left[-\eta\int_{p'=p}^{p_0}\frac{\mathrm{d}p}{p'v\xi_p\Sigma_s(p')}\right]. \tag{29}$$

Making use of

$$\exp(-a\eta) = \int_0^\infty \delta(t-a)\exp(-\eta)\,\mathrm{d}t \tag{30}$$

as well as of (1), (16), (23), we obtain for the sample-averaged number of particles of momentum p at time t

$$\overline{n}(p,t) = \frac{C}{\Sigma_\mathrm{s}(p)v(p)p\xi_p(p')}\exp\left(-\frac{1}{\overline{\tau}}f(p)\right)\delta(t-f(p)) \tag{31}$$

with

$$f(p) := \int_{p'=p}^{p_0} \frac{\mathrm{d}p'}{p'v(p')\xi_p(p')\Sigma_\mathrm{s}(p')}. \tag{32}$$

For simplicity, in (32) we have assumed the validity of (5), i.e., we have neglected trapping. We see that because of the δ-function in (31) the exponential function becomes $\exp(-t/\overline{\tau})$, in agreement with physical intuition.

Equations (31) and (32) may be simplified further by introducing the mean time between scatterings, τ_s, according to

$$\Sigma_\mathrm{s} = (v\tau_\mathrm{s})^{-1} \tag{33}$$

and noting that for narrow collision intervals we may write

$$\xi_p = -\frac{1}{p}\left(\frac{\mathrm{d}p}{\mathrm{d}t}\right)_\mathrm{s}\tau_\mathrm{s}, \tag{34}$$

where $-(\mathrm{d}p/\mathrm{d}t)_\mathrm{s}$ is the rate of momentum loss due to scattering. We thus obtain finally

$$\overline{n}(p,t) = \frac{n_0}{(\mathrm{d}p/\mathrm{d}t)_s}\exp(-t/\overline{\tau})\delta(t-f(p)) \tag{35}$$

with

$$f(p) = \int_{p_0}^{p} \frac{\mathrm{d}p'}{(\mathrm{d}p'/\mathrm{d}t)_\mathrm{s}}. \tag{36}$$

Equation (35) forms a suitable starting point for analysing AMOC (=age–momentum correlation) data on the slowing down of positronium that has been formed with kinetic energies that are large compared with $3k_\mathrm{B}T/2$ [16].

6. Weak anisotropy

Weak anisotropy refers to a property of the distribution of flight directions. It implies that the differential particle flux is well represented by

$$\Phi(\boldsymbol{r},\Omega,p;t) = \frac{1}{4\pi}\left[\Phi(\boldsymbol{r},p;t) + 3J(\boldsymbol{r},p;t)\cos\vartheta\right] \tag{37}$$

and that

$$J(\boldsymbol{r},p;t) \ll \Phi(\boldsymbol{r},p;t) \tag{38}$$

holds. In (37), $\cos\vartheta$ denotes the direction cosine of the flight direction Ω with respect to the z-axis of a suitably chosen polar coordinate system; $J(\boldsymbol{r},p;t)$ is the density of the particle current in the z-direction.

Unless the interaction leading to scattering is of extremely long range (as is, e.g., the Coulomb interaction), its description in terms of s and p scattering in the laboratory system as well as the assumption that $\mathbf{\Sigma}_{\mathrm{s}}(\mathbf{\Omega}' \to \mathbf{\Omega}, p' \to p)$ has rotational symmetry should be adequate. This means that we may write

$$\mathbf{\Sigma}_{\mathrm{s}}(\mathbf{\Omega}' \to \mathbf{\Omega}, p' \to p) = \frac{1}{4\pi}\left[\mathbf{\Sigma}_{\mathrm{s}}(p' \to p) + 3\mathbf{\Sigma}_{\mathrm{s}}^{(1)}(p' \to p)\cos\vartheta\right] \tag{39}$$

with

$$\mathbf{\Sigma}_{\mathrm{s}}^{(1)}(p' \to p) = 2\pi \int_{-1}^{+1} \mathbf{\Sigma}_{\mathrm{s}}(\mathbf{\Omega}' \to \mathbf{\Omega}, p' \to p)\cos\vartheta\ \mathrm{d}\cos\vartheta. \tag{40}$$

For later use we introduce the quantities

$$\mathbf{\Sigma}_{\mathrm{m}}(p' \to p) := \mathbf{\Sigma}_{\mathrm{s}}(p' \to p) - \mathbf{\Sigma}_{\mathrm{s}}^{(1)}(p' \to p), \tag{41}$$

called the macroscopic *differential* cross section for momentum transfer, and

$$\mathbf{\Sigma}_{\mathrm{m}}(p) = \int_0^\infty \mathbf{\Sigma}_{\mathrm{m}}(p' \to p)\ \mathrm{d}p', \tag{42}$$

the macroscopic *total* cross section for momentum transfer (also known as transport cross section).

Insertion of (37) and (39) into (10) gives us the following pair of coupled equations for the event density $\mathbf{\Psi}(\boldsymbol{r}, p; t)$ and the current density $J(\boldsymbol{r}, p; t)$:

$$\begin{aligned}
&\frac{1}{\left[\mathbf{\Sigma}_{\mathrm{s}}(p) + \mathbf{\Sigma}_{\mathrm{a}}(p)\right]v}\frac{\partial \mathbf{\Psi}(\boldsymbol{r}, p; t)}{\partial t} + \frac{\partial J(\boldsymbol{r}, p; t)}{\partial z} + \mathbf{\Psi}(\boldsymbol{r}, p; t) \\
&\qquad = \int_0^\infty \frac{\mathbf{\Sigma}_{\mathrm{s}}(p' \to p)}{\mathbf{\Sigma}_{\mathrm{s}}(p') + \mathbf{\Sigma}_{\mathrm{a}}(p')}\mathbf{\Psi}(\boldsymbol{r}, p'; t)\ \mathrm{d}p', \qquad (43)\\
&\frac{1}{\left[\mathbf{\Sigma}_{\mathrm{s}}(p) + \mathbf{\Sigma}_{\mathrm{a}}(p)\right]v}\frac{\partial J(\boldsymbol{r}, p; t)}{\partial t} + \frac{1}{3\left[\mathbf{\Sigma}_{\mathrm{s}}(p) + \mathbf{\Sigma}_{\mathrm{a}}(p)\right]^2}\frac{\partial \mathbf{\Psi}(\boldsymbol{r}, p; t)}{\partial z} + J(\boldsymbol{r}, p; t) \\
&\qquad = \int_0^\infty \frac{\mathbf{\Sigma}_{\mathrm{s}}^{(1)}(p' \to p)}{\mathbf{\Sigma}_{\mathrm{s}}(p') + \mathbf{\Sigma}_{\mathrm{a}}(p')} J(\boldsymbol{r}, p'; t)\ \mathrm{d}p'. \qquad (44)
\end{aligned}$$

The integral on the right-hand side of (43) may be evaluated as follows, making use of (11) and (19):

$$\begin{aligned}
&\int_0^\infty \frac{\mathbf{\Sigma}_{\mathrm{s}}(p' \to p)}{\mathbf{\Sigma}_{\mathrm{s}}(p') + \mathbf{\Sigma}_{\mathrm{a}}(p')}\mathbf{\Psi}(\boldsymbol{r}, p'; t)\ \mathrm{d}p' \\
&\qquad = \int_{p'=p}^{p'=p/\beta} \frac{\mathbf{\Sigma}_{\mathrm{s}}(p')}{\mathbf{\Sigma}_{\mathrm{s}}(p') + \mathbf{\Sigma}_{\mathrm{a}}(p')} g_p(p' \to p)\mathbf{\Psi}(\boldsymbol{r}, p'; t)\ \mathrm{d}p' \\
&\qquad = \frac{\partial \mathbf{\Xi}(\boldsymbol{r}, p; t)}{\partial p} + \frac{\mathbf{\Sigma}_{\mathrm{s}}(p)}{\mathbf{\Sigma}_{\mathrm{s}}(p) + \mathbf{\Sigma}_{\mathrm{a}}(p)}\mathbf{\Psi}(p). \qquad (45)
\end{aligned}$$

Because of the narrowness of the collision interval we are justified in replacing in the integrand in (45) p' by p except in the term $\mathbf{\Sigma}_{\mathrm{s}}^{(1)}(p' \to p)$. Laplace transforming (43) and (44) with respect to time results in the pair

$$\frac{\partial \tilde{J}(\boldsymbol{r}, p; \eta)}{\partial z} + \frac{\mathbf{\Sigma}_{\mathrm{a}}(p) + (\eta/v)}{\mathbf{\Sigma}_{\mathrm{s}}(p) + \mathbf{\Sigma}_{\mathrm{a}}(p)}\tilde{\mathbf{\Psi}}(\boldsymbol{r}, p; \eta) - \frac{\partial \tilde{\mathbf{\Xi}}(\boldsymbol{r}, p; \eta)}{\partial p} = \frac{\mathbf{\Psi}(\boldsymbol{r}, p; 0^+)}{(\mathbf{\Sigma}_{\mathrm{s}}(p) + \mathbf{\Sigma}_{\mathrm{a}}(p))v}, \tag{46}$$

$$\frac{1}{3(\mathbf{\Sigma}_{\mathrm{s}}(p) + \mathbf{\Sigma}_{\mathrm{a}}(p))}\frac{\partial \tilde{\mathbf{\Psi}}(\boldsymbol{r}, p; \eta)}{\partial z} + (\mathbf{\Sigma}_{\mathrm{m}}(p) + \mathbf{\Sigma}_{\mathrm{a}}(p) + (\eta/v))\tilde{J}(\boldsymbol{r}, p; \eta) = \frac{1}{v}J(\boldsymbol{r}, p; 0^+). \tag{47}$$

Differentiating (47) with respect to z and eliminating $\partial\tilde{J}/\partial z$ gives us

$$\frac{1}{3\left[\boldsymbol{\Sigma}_{\mathrm{s}}(p)+\boldsymbol{\Sigma}_{\mathrm{a}}(p)\right]\left[\boldsymbol{\Sigma}_{\mathrm{m}}(p)+\boldsymbol{\Sigma}_{\mathrm{a}}(p)+(\eta/v)\right]}\frac{\partial^2\tilde{\boldsymbol{\Psi}}(\boldsymbol{r},p;\eta)}{\partial z^2} - \frac{\boldsymbol{\Sigma}_{\mathrm{a}}(p)+(\eta/v)}{\boldsymbol{\Sigma}_{\mathrm{s}}(p)+\boldsymbol{\Sigma}_{\mathrm{a}}(p)}\tilde{\boldsymbol{\Psi}}(\boldsymbol{r},p;\eta)+\frac{\partial\tilde{\boldsymbol{\Xi}}(\boldsymbol{r},p;\eta)}{\partial p} = \frac{1}{(\boldsymbol{\Sigma}_{\mathrm{m}}(p)+\boldsymbol{\Sigma}_{\mathrm{a}}(p))v+\eta}\frac{\partial J(\boldsymbol{r},p;0^+)}{\partial z} - \frac{1}{(\boldsymbol{\Sigma}_{\mathrm{s}}(p)+\boldsymbol{\Sigma}_{\mathrm{a}}(p))v}\boldsymbol{\Psi}(\boldsymbol{r},p;0^+). \tag{48}$$

Using the Laplace-transformed equation (23), $\tilde{\boldsymbol{\Psi}}(\boldsymbol{r},p;\eta)$ may be replaced by $\tilde{\boldsymbol{\Xi}}(\boldsymbol{r},p;\eta)$. We thus have succeeded in deriving a linear parabolic differential equation for $\tilde{\boldsymbol{\Xi}}(\boldsymbol{r},p;\eta)$ with the special feature that its coefficients do not depend on the independent variable z. This feature allows us to transform (48) into a diffusion equation by changing the variables [17]. Since the general solution of the inhomogeneous equation (48) may be found by adding a particular solution to the general solution of the homogeneous equation, we concentrate on the latter equation.

With $\tilde{\boldsymbol{\Xi}}(\boldsymbol{r},p;\eta)$ as the dependent variable, the homogeneous equation following from (48) reads

$$\frac{\partial^2\tilde{\boldsymbol{\Xi}}}{\partial z^2}+3\boldsymbol{\Sigma}_{\mathrm{s}}(\boldsymbol{\Sigma}_{\mathrm{m}}+\boldsymbol{\Sigma}_{\mathrm{a}}+(\eta/v))p\xi_p\frac{\partial\tilde{\boldsymbol{\Xi}}}{\partial p}-3(\boldsymbol{\Sigma}_{\mathrm{m}}+\boldsymbol{\Sigma}_{\mathrm{a}}+\eta/v))(\boldsymbol{\Sigma}_{\mathrm{a}}+\eta/v)\tilde{\boldsymbol{\Xi}}=0. \tag{49}$$

The zero-order term in (49) may be removed by introducing as the dependent variable

$$\tilde{\chi}(\boldsymbol{r},p;\eta)=\tilde{\boldsymbol{\Xi}}(\boldsymbol{r},p;\eta)\exp\left[-\int\frac{\boldsymbol{\Sigma}_{\mathrm{a}}(p')+(\eta/v(p'))}{\boldsymbol{\Sigma}_{\mathrm{s}}(p')p'\xi_p(p')}\,\mathrm{d}p'\right]. \tag{50}$$

Choosing

$$s=\frac{1}{3}\int_p^{p_0}\frac{\mathrm{d}p'}{p'\xi_p(p')\boldsymbol{\Sigma}_{\mathrm{s}}(p')[\boldsymbol{\Sigma}_{\mathrm{m}}(p')+\boldsymbol{\Sigma}_{\mathrm{a}}(p')+(\eta/v(p'))]} \tag{51}$$

as the independent variable and going back to three space dimensions gives us finally

$$\partial\tilde{\chi}(\boldsymbol{r},p;\eta)/\partial s=\nabla^2\tilde{\chi}(\boldsymbol{r},p;\eta). \tag{52}$$

This is the well-known diffusion (or heat-conduction) equation. Thus, all of the analytical and computational techniques developed for solving this equation for given initial and boundary conditions are available for the slowing-down problem of light particles, provided that the conditions stated at the beginning of this section are satisfied.

The basic ideas of the present section were developed for treating the slowing down of neutrons [7, 8, 10, 12]. In its simplest form (stationary state, absorption cross section $\boldsymbol{\Sigma}_{\mathrm{a}}$ small compared with the scattering cross section $\boldsymbol{\Sigma}_{\mathrm{s}}$), equation (52) may be written as

$$\frac{\partial\boldsymbol{\Xi}}{\partial s}-\nabla^2\boldsymbol{\Xi}=0 \tag{53}$$

with

$$s=\int_E^{E_0}\frac{l_{\mathrm{m}}(E')l_{\mathrm{s}}(E')}{3\xi_E(E')E'}\,\mathrm{d}E'. \tag{54}$$

Here, in accordance with the usage in neutronics, the kinetic energy E has been introduced as a variable of integration and the macroscopic cross sections have been replaced by the corresponding mean free paths (cf. section 2 and equation (55)). ξ_E is the average logarithmic energy loss per collision, which in the non-relativistic case is related to ξ_p by

$\xi_E = 2\xi_p$. In neutronics, $s = s(E)$ is called the 'age' of neutrons that were slowed down from an initial energy E_0 to the energy E, presumably because of the analogy of s with the time-variable in diffusion problems. In the present context we refrain from using this terminology for two reasons.

(i) For positrons, 'age' is used for the time that the e^+ have spent in the sample when they annihilate, irrespective of what their energy is at that moment (cf. section 5).

(ii) s does not have the dimension of time but of a length squared. As will be demonstrated below, apart from a proportionality factor s is the mean square displacement that the particles have undergone during slowing down from the initial energy E_0 to the energy E. Nevertheless, for historical reasons the theory developed in this section will be referred to as 'Fermi's theory of aging' or, for short, 'age theory'.

If we introduce the mean time between scattering events, τ_s, according to

$$l_s = v\tau_s \tag{55}$$

we may write the average logarithmic energy loss per collision as

$$\xi_E = -\frac{1}{E}\left(\frac{dE}{dt}\right)_s \tau_s, \tag{56}$$

where $(dE/dt)_s$ denotes the rate of energy loss by scattering. Inserting (55), (56) into (54) gives us

$$s = -\int_{E'=E}^{E_0} \frac{v(E')l_m(E')}{3(dE'/dt)_s}\, dE' = \int_{E_0}^{E} \frac{D(E')}{(dE'/dt)_s}\, dE'. \tag{57}$$

In (57) we have made use of the expression

$$D(E) = vl_m/3 \tag{58}$$

for the diffusivity D of the particles. In the non-relativistic limit we may write, for particles of mass m,

$$s = -\frac{2}{3m}\int_{E'=E}^{E'=E_0} \frac{E'\tau_m(E')}{(dE'/dt)_s}\, dE', \tag{59}$$

where

$$\tau_m = v/l_m \tag{60}$$

is the relaxation time for momentum relaxation.

In the presence of internal particle sources, a source term has to be added on the right-hand side of (53). Let us assume that in an unbounded space there is a particle source at $\boldsymbol{r} = 0$ and nowhere else, and that this source emits particles with a well-defined kinetic energy E_0. Then the solution of (53) with the normalization

$$\int \Xi(\boldsymbol{r}, E; E_0)\, d^3\boldsymbol{r} = 1 \tag{61}$$

is [17]

$$\Xi(\boldsymbol{r}, E; E_0) = (4\pi s)^{-3/2} \exp(-r^2/4s). \tag{62}$$

From (62) it follows that

$$\langle r_\Xi^2 \rangle := \int r^2 \Xi(\boldsymbol{r}, E; E_0)\, d^3\boldsymbol{r} = 6s. \tag{63}$$

Hence in this case $6s$ has the physical meaning of the mean square of the distance over which the particles slow down to E from their starting energy E_0. (The integration in (61) and (63) extends over all space.)

7. An application of age theory: slowing down by optical phonon scattering

For light particles such as positrons, the theory developed in section 6 is general. It may be applied to any slowing-down mechanism satisfying the conditions of validity set out in section 6. As an example, we shall treat the slowing down due to scattering by optical phonons described by Einstein's model.

Einstein's model postulates that the motion of the atoms in condensed matter can be described by phonons with a frequency ω_{op} that is independent of the phonon wavenumber. The notation ω_{op} alludes to the fact that the Einstein model often provides a good description of so-called 'optical phonons', i.e. of those phonon modes whose frequency approaches a finite value when the phonon wavenumber approaches zero. Within the framework of this model it is natural to describe the coupling between the particles and the phonons by a wavenumber-independent deformation–potential parameter, E_{op}.

In the model just outlined, the scattering probability is independent of the flight directions before and after scattering, and hence of the scattering angle ψ. This permits the transport equation to be solved exactly if spatial homogeneity is assumed, i.e., if the field variables are independent of $\boldsymbol{r}$ [18]. In a material of density ρ, for particles of mass m the inverse of the momentum relaxation time, τ_m^{-1}, and the normalized energy loss rate, $-\mathrm{d}\varepsilon/\mathrm{d}t$, are given by†

$$\left.\begin{array}{c}\tau_m^{-1}\\ -\mathrm{d}\varepsilon/\mathrm{d}t\end{array}\right\} = \left(\frac{m}{2}\right)^{3/2} \frac{E_{op}^2 \,\mathrm{cosech}(\hbar\omega_{op}/2k_B T)}{\pi\rho\hbar^2(\hbar\omega_{op})^{1/2}} [A\,\mathrm{Re}(\varepsilon-1)^{1/2} \pm A^{-1}(\varepsilon+1)^{1/2}] \qquad (64)$$

with the abbreviations

$$\varepsilon := E/\hbar\omega_{op} \qquad A := \exp(\hbar\omega_{op}/2k_B T). \qquad (65)$$

For $\varepsilon \geqslant 1$, it follows from (64) that

$$-\frac{1}{\tau_m}\frac{\mathrm{d}\varepsilon}{\mathrm{d}t} = \frac{m^3 E_{op}^4 \,\mathrm{cotanh}(\hbar\omega_{op}/2k_B T)}{2\pi^2\rho^2\hbar^5\omega_{op}} \left\{\varepsilon - \varepsilon^*\right\} \qquad (66)$$

with

$$\varepsilon^* := \mathrm{cotanh}(\hbar\omega_{op}/k_B T) =: E^*/\hbar\omega_{op}. \qquad (67)$$

Inserting (66) into (59) gives us the mean square of the slowing-down distance as a function of the kinetic energy E as

$$\begin{aligned} 6s &= \frac{\hbar\omega_{op}}{mB^2}\tanh\left(\frac{\hbar\omega_{op}}{2k_B T}\right)\int_{\varepsilon'=\varepsilon}^{\varepsilon'=E_0/\hbar\omega_{op}} \frac{\varepsilon'}{\varepsilon'-\varepsilon^*}\,\mathrm{d}\varepsilon' \\ &= \frac{1}{mB^2}\tanh(\hbar\omega_{op}/2k_B T)\left\{E_0 - E + E^*\ln\left(\frac{E_0-E^*}{E-E^*}\right)\right\} \end{aligned} \qquad (68)$$

with

$$B := \frac{m^{3/2}(E_{op}/\hbar)^2}{2\pi\rho(2\hbar\omega_{op})^{1/2}}. \qquad (69)$$

Of the parameters appearing in (68), ω_{op} and thus E^* (cf. (67)) may be deduced from optical or specific-heat data on the material under consideration. In the application to positronium, m is twice the electron mass, m_e. The quantities E_0 and B are related to the

† It may appear puzzling that the energy loss rate is obtained by multiplying by $\pm\hbar\omega_{op}$ the phonon absorption and emission terms in the expression for τ_m^{-1} rather than that for τ_s^{-1}. The explanation is that in the present case the effect of the weight factor $(1-\cos\psi)$ (ψ = scattering angle) in the momentum relaxation rate cancels by symmetry, so $\tau_s = \tau_m$.

formation and slowing down of Ps, E_0 being the (average) initial kinetic energy of Ps. If the condition $E \gg E^*$ is satisfied, the relationship

$$E^{1/2} = E_0^{1/2} - (\hbar\omega_{op})^{1/2} Bt \tag{70}$$

holds, where t is the time that has passed since the Ps was formed [3]. Making use of the relationship $E^{1/2} = (2m)^{-1/2} p$, where p is the momentum of the annihilating electron positron pairs, the AMOC technique [16] allows us to determine the t-dependence of the p-distribution and to deduce from this both E_0 and $B(\hbar\omega_{op})^{1/2}$, provided that they lie in the ranges accessible to the technique. If we use (70) to define a slowing-down time

$$t_{sd} = B^{-1}(E_0/\hbar\omega_{op})^{1/2} \tag{71}$$

and insert (71) into (68), we obtain

$$6s = \frac{\hbar\omega_{op}}{m} t_{sd}^2 \tanh(\hbar\omega_{opt}/2k_B T)\left(1 - \frac{E}{E_0} + \frac{E^*}{E_0}\ln\frac{E_0 - E^*}{E - E^*}\right). \tag{72}$$

With $m = 2m_e$ and, as typical values for Ps-forming materials, $2\pi\omega_{ops} = 1 \times 10^{14}$ s^{-1} and $t_{sd} = 25 \times 10^{-12}$ s [16], the square root of the numerical prefactor in (72) becomes

$$(\hbar\omega_{op} t_{sd}^2/m)^{1/2} = 4.8\ \mu\text{m}. \tag{73}$$

With the further assumptions $\rho = 1 \times 10^6$ kg m^{-3} and $E_0 = 6.8$ eV, the relationship

$$(E_{opt}/\hbar)^2 = 2\pi\rho(2E_0)^{1/2} m^{-3/2} t_{sd}^{-1} \tag{74}$$

gives us for the parameter characterizing the deformation potential

$$E_{op} = 0.3 \times 10^{10}\ \text{eV m}^{-1}. \tag{75}$$

This means that a displacement of the host atoms by 10^{-10} m changes the positron energy by 0.3 eV, which is certainly a plausible order of magnitude, indicating that the model [3] is capable of accounting for the slowing-down observations on Ps-formers with optical phonons.

The preceding treatment disregards the position annihilation. Often this is a good approximation since, unless $\Sigma_a \ll \Sigma_s$, one cannot study the slowing-down process in detail. In the present case the quadratures required for taking into account Σ_a in calculating the Laplace transform $\tilde{\Xi}$ may be performed in closed form by the procedure developed in [3]. However, since the resulting expressions are fairly complicated we refrain from giving them here. For moderately large Σ_a the energy $\check{E}$ at which (68) has to be cut off because of the finite mean lifetime $\overline{\tau}$ of the e^+ may be estimated simply from

$$\overline{\tau} = \int_{E'=E_0}^{E'=\check{E}} \frac{1}{(\mathrm{d}E'/\mathrm{d}t)_s}\ \mathrm{d}E'. \tag{76}$$

The integral has been evaluated in the appendix of reference [3].

The present numerical example corresponds to $(E_0/\hbar\omega_{op})^{1/2} = 4.0$ and, if we attribute to p-Ps the mean vacuum lifetime $\overline{\tau} = 1.25 \times 10^{-10}$ s, to $B\overline{\tau} = 20$. This means that in this case taking into account Σ_a would modify equations (68) and (70) only slightly. On the other hand, the estimate $t_{sd} \simeq \overline{\tau}/5$ indicates that in calculating the mean square slowing-down distance $6s = \langle r_\Xi^2 \rangle$, the mechanisms limiting the diffusivity of *thermalized* Ps, in particular the scattering by acoustical phonons, must be allowed for. Nevertheless, the numerical estimate (73) in conjunction with (72) indicates that for Ps $\langle r_\Xi^2 \rangle$ is much larger than the extension of the spur or the 'short track' discussed in models of Ps formation (see, e.g., [19]). It appears that so far this aspect of Ps formation has not received adequate attention.

A noteworthy feature of (68) and (69) is that the mean displacement $(6s)^{1/2}$ is proportional to m^{-2}. This has the consequence that for muonium Mu $= (\mu^+ e^-)$, with $m = 103 m_e$, the numerical value (73) is about four powers of ten smaller than for Ps (in the present example, equal to 0.45 nm). This means that a fair fraction of Mu 'atoms' will interact with the spur produced by their own μ^+ before they formed Mu, in striking contrast to the case for Ps.

Acknowledgments

Most of the work reported in the present paper was done during the author's stay at the University of Cape Town as awardee of a South African–German Humboldt award. He would like to gratefully acknowledge the hospitality of the staff of the Department of Physics of the UCT, in particular that of Dr David Britton and Professor Jean Cleymans.

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