Monte Carlo studies of positrons in matter. Temperature and electric field effects on lifetime spectra in low-temperature, high-density helium gas

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Lifetime spectra of slow positrons in helium gas at low temperatures and high densities have been calculated using a Monte Carlo technique. Spectra are calculated both with and without applied electric fields using a two-parameter model based on the picture of helium cluster or droplet formation around the positron. The model is remarkably successful in reproducing the observed peak in the low-temperature spectra, the changes in the peak with variation of temperature and electric field, and the behavior of the "equilibrium" decay rate under a variety of conditions. At 5.5°K, the optimal model parameters, independent of electric field, are found to be $E_R = 0.005$ eV for the threshold energy of droplet formation, and $Z_R = 18.2$ for the enhanced decay-rate parameter. The simple slowing-down approximation is relatively successful in explaining the high-temperature spectra and in predicting the position of the peak in the low-temperature spectra when no electric field or only very small fields are present. The approximation breaks down at low temperatures and high electric fields, and consideration of the average positron energy and the width of the energy distribution as functions of time shows why this breakdown occurs.

I. INTRODUCTION

In a recent paper[1] (hereafter referred to as paper I), we developed a Monte Carlo technique for simulating the behavior of positrons in matter and applied that method to the calculation of lifetime spectra of slow positrons in helium gas at temperatures ranging from 77 to 1000 °K. The results obtained in paper I were in excellent agreement both with experiment and with calculations[2] performed using the diffusion equation approach.[3] We argued that the Monte Carlo method lends itself exceedingly well to the study of a variety of phenomena involving positrons, including many cases in which application of the diffusion equation or other theoretical techniques is difficult, if not impossible.

In this paper, we use the Monte Carlo approach to investigate the behavior of positrons in high-density helium gas at temperatures only a few degrees above the condensation point. Under these conditions, new features appear which are not present in the high-temperature spectra discussed earlier. In particular, variations in temperature and/or electric field, which produce little if any effect at higher temperatures, cause dramatic changes in both the equilibrium decay rate[4] and the height and location of the peak (see Fig. 1) in the low-temperature lifetime spectra. The peak itself is present only at low temperatures and high densities. It has been attributed[5] to the formation of clusters or droplets of helium about individual positrons, and recent experimental[6] and theoretical[7] studies have provided more rigorous support for this view.

Before describing the results of our calculations, we first give a brief summary of the relevant experimental results and an account of the computational techniques employed. In the final sections, we present the results of our calculations and discuss the implications of our findings for the study of positron-helium as well as other positron-gas systems.

II. SUMMARY OF EXPERIMENTAL RESULTS

Positron-annihilation lifetime spectra (rate of annihilation versus time between emission of positron into the sample and annihilation) in gases can generally be resolved into three components.

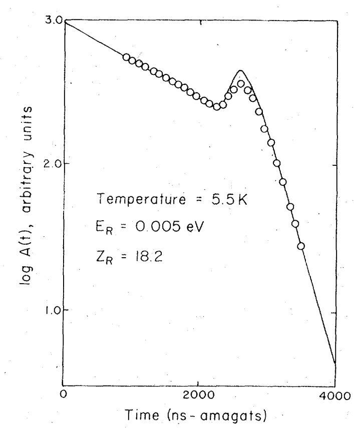

FIG. 1. Lifetime spectra for slow positrons in high-density helium gas at 5.5°K. Parameters in σ_a: E_R =0.005 eV, Z_R=18.2. Non-sink-like model. Solid line, calculated, present work. Circles, experimental, Canter *et al.*, Ref. 10.

The first, or "prompt" component results primarily from the annihilation of positrons which either form parapositronium or are stopped by the solid parts of the apparatus. A second component may be identified with the annihilation of positrons which form orthopositronium. The prompt component is present only at very short times, while the orthopositronium component of the spectrum is essentially a pure exponential which persists to extremely long times. On removing these two components, as well as a flat background contribution due to uncorrelated coincidences from the experimental spectrum, one is left with the spectrum of the so-called "slow" positrons, i.e., those which have lost sufficient energy that they are energetically incapable of forming positronium by removal of an electron from an atom of the gas. It is these slow positrons which provide the most illuminating probe of the interactions between the gas and the positron.

As discussed in paper I, the chief features of high-temperature slow positron lifetime spectra in helium gas are a broad shoulder, which results from the appearance of a minimum in the momentum-transfer cross section, and a pure-exponential long-time behavior, attributed to the positrons having reached their equilibrium-energy distribution. When Roellig and co-workers[8-10] investigated the lifetime spectra in helium at temperatures as low as 4.6 °K, several new phenomena emerged. The most notable of these features was the appearance of a peak in the annihilation spectrum shortly after the shoulder region. This peak is seen only below a temperature T_H, and this temperature increases with increasing density of the gas.[10] Hautojärvi *et al.*[6] have recently obtained experimental data which support the interpretation of T_H as the temperature of a gas-liquid-like phase transition in the neighborhood of the positron. The critical temperature (maximum value of T_H) for this transition is somewhat higher than for the ordinary gas-liquid transition [$T_H^{\max} = 6.6$ K (8.4 K), $T_C = 3.3$ K (5.3 K) for ^{3}He (^{4}He)], while the critical density is the same for both the positron-induced and the ordinary condensation [$\rho_C = 0.90 \pm 0.05 (1.00 \pm 0.05)$ cm^{-3} for ^{3}He (^{4}He)]. As the temperature is increased toward T_H, the peak moves to longer times and becomes less pronounced until, at T_H, it disappears. Above T_H, changes in temperature have little perceptible effect on the spectrum.[1] Quantum-mechanical[7] and semiclassical[11] calculations are in general agreement with Hautojärvi's experiments,[6] and suggest that the droplets should begin to form with an initial radius of 10–15 Å, i.e., about 100–200 helium atoms.

The temperature and density dependences of the equilibrium annihilation rates λ_e also differ significantly from their counterparts in high-temperature helium spectra. At high temperature, λ_e decreases very slowly with temperature and is directly proportional to the density. In contrast, at temperatures below T_H, λ_e falls rapidly (by a factor of about 5 within one degree) with increasing T and reaches a constant value as density is increased at constant temperature.[10] These results are also consistent with the cluster model[6,7,10] and cannot be explained by the positron–single-helium-atom interaction picture which appears to account satisfactorily[1] for the high-temperature spectra.

Since positrons are charged particles, one might expect that carrying out experiments involving positrons in electric fields would shed additional light on the phenomena involved. Positron-annihilation lifetime spectra for helium have been measured in electric fields both at high[12-14] and at low[9] temperatures. The high-temperature spectra are affected only very slightly even by fields as large as 1350 V cm^{-1} amagat^{-1}. In contrast, the low-temperature spectra undergo significant changes when electric fields are applied. Two principal effects are observed as the applied field is increased. First, the peak in the spectrum becomes lower and broader, though no appreciable shift in its location is observed. Secondly, the equilibrium decay rate drops sharply until it reaches a constant value. The rate of decrease of λ_e with electric field is greatest at low densities and at low temperatures.

III. METHOD OF CALCULATION

A. Field-free spectra

The method used to calculate the annihilation spectra of positrons in helium in the absence of electric fields is identical to that outlined in paper I. We recall that trajectories are simulated for positrons having momentum-dependent annihilation and elastic (momentum-transfer) cross sections σ_a and σ_e, respectively. A key element of the method is that instead of following individual positrons, we track a *swarm* of positrons having identical momenta, and allow a fraction $\sigma_a/(\sigma_a + \sigma_e)$ of the swarm to annihilate at each collision. This procedure markedly increases the efficiency of the calculation, since otherwise each positron would have to collide an average of about 10 000 times before annihilating. The initial distribution of slow positrons, which was found in paper I to have a negligible effect on the lifetime spectrum, is chosen as the uniform distribution in momentum space below the Ore gap (i.e., $E \leq 17.7$ eV). For the velocity-dependent cross sections σ_e and σ_a, we again use the analytic expressions given by Humberston,[2,15] although the annihilation cross section σ_a has been modified to account for new low-temperature phenomena in a manner to be described below. The phase shifts required to calculate the angular distribution of elastically scattered positrons are obtained from the calculations of Humberston[15] as described in paper I.

While the calculated cross sections and phase shifts appear adequate to account for the high-temperature lifetime spectra,[1] they fail to produce the peak seen in the spectra at low temperatures. In view of the strong evidence for cluster formation at low temperatures,[6,7] it seems reasonable to modify the cross sections to take account of this phenomenon. A simple and physically reasonable model, which affects only the annihilation cross section σ_a, has been suggested by Tao and Kelly.[16] In this model, cluster formation has the effect of producing a sharp increase in σ_a when the positron energy falls below a critical value E_R.

The model as employed in our low-temperature calculations consists of a two-parameter modification[16] of the single-atom annihilation cross section,[1,15] together with the elastic-scattering cross section and phase shifts used in our high-temperature work.[1] Our annihilation cross section is given by

$$\sigma_a(v)=\begin{cases}\bar{\sigma}_a(v), & v>v_R\,,\\ \lambda_R/\rho v_R, & 0\leqslant v\leqslant v_R\,,\end{cases} \tag{1}$$

where $\bar{\sigma}_a$ is the calculated high-temperature cross section,[2] ρ is the number density of positrons, and λ_R is chosen as the equilibrium decay rate λ_e at the actual experimental temperature in the absence of electric fields. In the cluster picture, the threshold velocity v_R ($E_R=\frac{1}{2}mv_R^2$) characterizes the strength of the interactions which hold the cluster together. More specifically, E_R is the greatest energy a positron may have at the given temperature and gas density in order that a cluster may form about the positron. We also define $Z_i=(\pi r_0^2 c\rho)^{-1}\lambda_i$, where $i=e$ or R. That is, Z_R is the effective number of electrons "seen" by a positron within a cluster.

The quantities λ_e and Z_e, like the time of appearance of the peak, are determined by analysis of the experimental (or calculated) spectrum. The quantities λ_R, Z_R, and v_R, on the other hand, are parameters in our model, initially chosen to give good agreement with the field-free experimental spectra.[17]

In Sec. III, we discuss how these parameters change with temperature and applied field. While Eq. (1) clearly misrepresents the detailed shape of σ_a below v_R, we find that the annihilation spectra are far more sensitive to the behavior of σ_a in the immediate region of the threshold than to its variation at lower velocities. Given the quality of the available experimental data and the ambiguity of the theoretical models, we have chosen to use the relatively simple expression (1) rather than introduce additional empirical parameters into our cross section.

In addition to the annihilation rates, we also calculate for each channel an average positron energy and the "width" of the positron energy distribution. The average energy, which plays a key role in the so-called "slowing-down approximation",[18] is defined in our calculation as

$$\langle E_i\rangle=\frac{\sum_{j=1}^{N}\sum_{k=0}^{n_j(i)}(t_{j,k+1}-t_{j,k})E_{jk}n_{jk}}{\sum_{j=1}^{N}\sum_{k=0}^{n_j(i)}(t_{j,k+1}-t_{j,k})n_{jk}}\,, \tag{2}$$

where the calculation contains N positron swarms, and the jth swarm undergoes $n_j(i)$ collisions in the ith channel at times $t_{j1},\ t_{j2},\cdots,t_{jn_j(i)}$. The times t_{j0} and $t_{jn_j(i)+1}$ are defined as the initial and final times in the ith channel. During the interval between collisions k and $k+1$, the n_{jk} positrons remaining in the jth swarm all have energy E_{jk}.

The energy width is defined as

$$\Delta E_i=[\langle E_i^2\rangle-(\langle E_i\rangle)^2]^{1/2}\,, \tag{3}$$

where $\langle E_i\rangle$ is calculated as in Eq. (2) and $\langle E_i^2\rangle$ is obtained by replacing E_{jk} by E_{jk}^2 in the numerator of the right-hand side of Eq. (2). This quantity will be of considerable interest in our later discussions of the validity of the slowing-down approximation and of the differences between calculations performed with and without external electric fields.

B. Spectra in electric fields

The addition of an applied electric field to the problem affects only a single major aspect of the Monte Carlo calculation, the computation of the free time between successive collisions. However, this modification turns out to be far from trivial to implement, as we shall see below.

The calculations with electric fields point up one major advantage of the Monte Carlo over the diffusion equation approach. In the Monte Carlo calculation, the elastic scattering cross section we employ is the full, anisotropic, differential cross section. No feasible way has been found to use this expression in the diffusion equation, and an average, isotropic momentum-transfer cross section is generally assumed. While this approximation should have little adverse effect on field-free calculations, where the system is effectively isotropic, it may have more serious effects when the presence of a field makes the direction of motion of the positron a significant variable.

In general, for positrons with velocity $\vec{v}(t)$, number density ρ, and total cross section $\sigma(v)$ $(\sigma=\sigma_a+\sigma_e)$, the probability $P(\tau)$ of a free time greater than τ is given by

$$P(\tau)=\exp\left(-\int_{t=0}^{\tau}\rho v(t)\sigma[v(t)]\,dt\right), \tag{4}$$

where the time t is measured from the previous collision and $v(t)$ is the magnitude of the vector $\vec{v}(t)$. The correct distribution of free times is simulated by choosing a random number r uniformly distributed between 0 and 1, setting $P(\tau)=r$, and solving for τ.[19] When there are no applied fields, $\vec{v}(t)=\vec{v}$ is constant between collisions, and we have simply

$$P(\tau)=\exp[-\rho v\sigma(v)\tau]=r,$$

which is easily solved to yield

$$\tau=-\ln r/[\rho v\sigma(v)]. \tag{5}$$

When nonzero fields are present, $\vec{v}(t)$ is not constant between collisions, and Eq. (5) is no longer valid. We now have

$$v(t)=|\vec{v}_0+\vec{a}t|,$$

where $\vec{v}_0$ is the positron velocity after the previous collision and $\vec{a}=e\vec{E}/m$ is the acceleration caused by the electric field $\vec{E}$, where e and m are the charge and mass of the positron. In principle, one should now choose the random number r, calculate the integral (4) as a function of τ and choose τ as the smallest value which makes $P(\tau)=r$.[20] The vector nature of $\vec{v}$, the possible existence of multiple roots, and especially the fact that σ is rarely known in a form that permits analytic integration of Eq. (4), all contribute to making such a procedure computationally unattractive. An alternative scheme which is considerably more efficient has been formulated by Skullerud.[21]

We present here a brief summary of Skullerud's method as adapted for the present study. Define the collision frequency of the positron $\nu(v)$ as

$$\nu(v)=\rho v\sigma(v). \tag{6}$$

Now choose a trial collision frequency $\nu'(v)$ such that $\nu'(v)$ is piecewise constant (a step function) and $\nu'(v)\geq\nu(v)$ for all velocities v. Thus, we replace the actual collision frequency ν by one which is always higher and which is independent of v except at a finite number of jump discontinuities.

The calculation now proceeds as follows. After the last collision, the positron has velocity $\vec{v}_0$. Using the constant collision frequency $\nu_0'=\nu'(v_0)$, calculate the time to the next collision. This is easily done, and we find

$$\tau=-\ln r/\nu_0'$$

as in Eq. (5). If all our values of τ are chosen in this way, we, of course, will grossly underestimate the mean-free time, since we have used the constant collision frequency ν_0' instead of the correct frequency $\nu[v(t)]$. We must therefore make two types of corrections. First, if as assumed[21] $\nu[v(t)]\leq\nu_0'$ for all t such that $0\leq t\leq\tau$, then we must "neglect" a fraction

$$f=1-\nu[v(\tau)]/\nu_0'$$

of the "collisions." For example, if $\nu[v(\tau)]/\nu_0'=0.25$, then choose a random number s uniformly distributed between 0 and 1. If $s<0.25$, the collision "occurs" at time τ. If $s\geq0.25$, then the free time is increased by τ, the trial-collision frequency is changed to $\nu'[v(\tau)]$, and the positron continues on its way with velocity $v(\tau)$, i.e., a new random number is chosen and the procedure is iterated. If, on the other hand, it is found that $\nu[v(t)]>\nu_0'$ for some t in the interval $0\leq t\leq\tau$, then the first value[20] of t for which the frequencies are equal is found, the positron is "brought back" to this time, ν_0' is set to ν_0 at the corresponding velocity and the positron is allowed to continue, starting from those values of $\vec{v}$ and τ.

The Skullerud procedure, though considerably slower than the simple Eq. (5) is quite accurate and relatively rapid, particularly if some care is taken to choose ν' so that as many positrons as possible approach but do not quite reach the collision frequency ν_0' before collision. Some experimentation is required to find the optimal form for ν_0', but our experience suggests that time spent in this search is well worthwhile.

Two other minor additions to the field-free calculation should also be noted. First, the presence of an external field requires that the direction of the positron's velocity with respect to the field direction be monitored. A field-free calculation uses only the magnitude of the velocity. Also, since the positron is subject to the acceleration of the field during the "free" time between collisions, its velocity must be updated immediately before as well as immediately after each collision.

The computer time required for a typical positron swarm increased significantly with the applied field strength, ranging from about 7 min at zero field to about 9 min at 0.4 V cm^{-1} amagat^{-1} on the Brandeis PDP-10 computer. We note that storage requirements are minimal (<10K words).

IV. RESULTS

A. Effects of electric field at high temperature

The first experimental studies[12-14] of positron annihilation in helium gas under the influence of

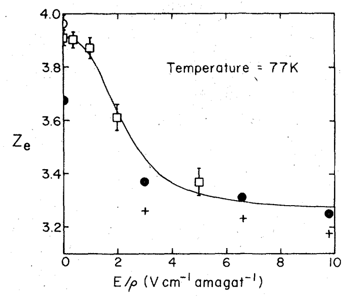

FIG. 2. Calculated values of Z_e at 77°K. Solid curve represents calculation (Ref. 2) based on diffusion equation. □, present work; ●, +, experimental, Leung and Paul, Ref. 12 (these values represent different analyses of the same data).

external electric fields were carried out at room temperature and at 77 °K. In order to test the effectiveness of our computational technique for dealing with positrons in electric fields, we first undertook to simulate some of these experiments as well as the accurate diffusion equation calculations of Campeanu and Humberston.[2] The calculations were carried out using the cross sections[2,15] employed in paper I without further modification. The shapes of the spectra obtained were in good agreement with experiment, and the values of Z_e shown in Fig. 2 suggest that our calculations are quantitatively reliable as well.

The small decrease in Z_e with increasing field may be understood by an argument based upon the slowing-down approximation. In this view, Z_e is simply the value corresponding to the average energy of a positron after equilibrium is reached. Increasing the electric field at a fixed temperature raises this equilibrium energy, just as raising the temperature would. Since Z_e is a decreasing function of energy in this energy range (see Fig. 3 of paper I), an increase in the equilibrium energy results in a decrease in Z_e. A similar small decrease in Z_e is also found[1] as the temperature is raised at values above $T = 77$ °K when no fields are present.

B. Low-temperature results

If one carries out Monte Carlo simulations of positron-annihilation spectra in helium at low temperatures using the same cross sections employed in the high-temperature studies, significant disagreement is found between the calculated and experimental spectra. The principal discrepancies are the absence of the peak described earlier (see Fig. 1) in the calculated spectrum and calculated values of Z_e which are four to five times lower than experiment.

Our model for the positron-helium interaction at low temperatures is given by the two-parameter modification of σ_a in Eq. (1). Although it is clearly an oversimplification, the excellent agreement it affords with experiment as well as the limited quantity and accuracy of data available for comparison suggest to us that introduction of additional parametric complexity at this time would only obscure the insights we seek. We have, however, considered one additional variation in the model. Depending upon the physical origin of the sharp increase in the annihilation cross section below v_R, this region of velocity space may be either "non-sink-like" or "sink-like" in nature. That is, positrons which enter this region may or may not be allowed to diffuse back out before annihilating.

In addition to showing that the experimental data are well described by our model, the results presented in this section deal with the question of how the parameters v_R and λ_R depend upon temperature and electric field in low-temperature, high-density helium. We first discuss how the spectra change as the temperature is varied in the absence of an external field. Then we look at the effects of increasing the field at constant temperatures.

1. Variation of temperature at zero field

In Fig. 1 we show a typical low-temperature zero-field spectrum calculated using our Monte Carlo program with σ_a given by Eq. (1). The experimental spectrum,[10] which is also shown, is in excellent agreement with our calculation. The peak in the calculated spectrum appears slightly too sharp, but this difference would be reduced or possibly eliminated by inclusion of the experimental time resolution in our calculation. As the temperature is increased, it is observed experimentally that Z_e decreases, while the peak in the spectrum becomes less pronounced and occurs at later times.[10] Given the correspondence between λ_R and λ_e in our model, the data unequivocally imply that λ_R is a decreasing function of temperature.

The dependence of v_R on temperature is somewhat more difficult to extract. The detailed treatments of the cluster model[6,7,10] make no direct prediction. Qualitatively, for any fixed positron velocity there should be an upper limit on the gas temperature at which clusters will be stable. That is, one should probably expect v_R to decrease with increasing temperature, though it is not at all clear how strong this dependence should be.

The average energy transfer per elastic collision increases with the difference between the positron energy and the thermal (helium) energy. Therefore, at higher temperatures, a typical posi-

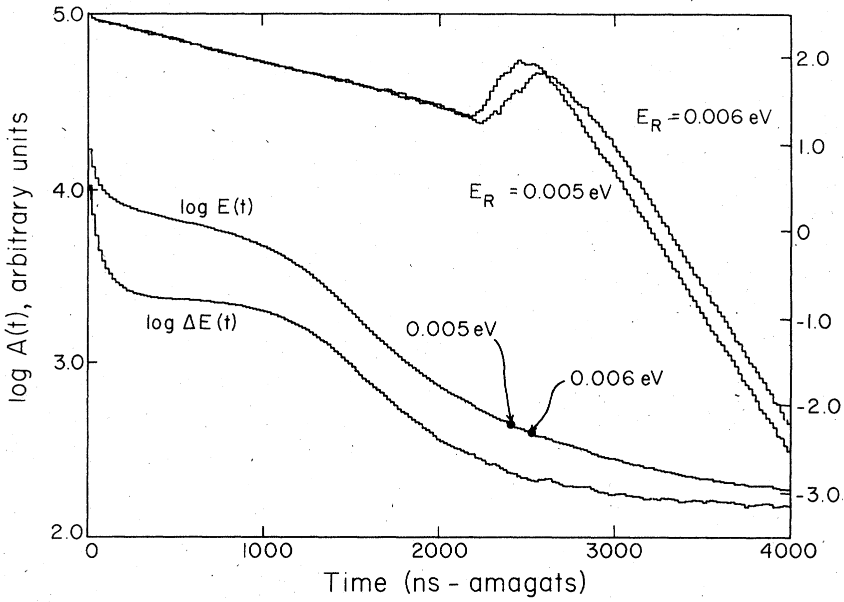

FIG. 3. Lifetime spectra at 5.5 °K calculated using $E_R = 0.005$ eV and $E_R = 0.006$ eV. Non-sink-like model $Z_R = 18.2$. Average positron energy $E(t)$ and width $\Delta E(t)$ are also shown (right-hand scale). Arrows indicate points at which $E(t) = 0.005$ eV and $E(t) = 0.006$ eV.

tron will lose energy more slowly and will reach any given E_R at a later time. Thus, the slowing-down approximation is qualitatively consistent with the observed change in the location of the peak even if v_R is temperature independent. However, our calculations show that the shift in the peak which occurs when v_R is kept constant as the temperature is increased is extremely small, almost zero, in contrast to the much larger shift observed experimentally.

The above results imply that v_R must decrease with temperature in order for a typical positron to require increasingly longer times to slow down to v_R at higher temperatures. One might argue, however, that this conclusion is crucially dependent upon our choice of the elastic scattering cross section which determines the rate of slowing down of the positron. In order to provide at least a partial test of this hypothesis, we recalculated the spectra at various temperatures using a cross section $\sigma_e'(v) = 2\sigma_e(v)$. As expected, the new cross section causes the positrons to slow down twice as rapidly, and for a given value of v_R the peak appears at a time half as great as before. However, if one uses σ_e', chooses v_R to give agreement with experiment at one temperature, and then employs this same v_R to calculate the spectrum at a higher temperature, the shift in the peak is still grossly underestimated. Since the shape of $\sigma_e(v)$, if not the exact magnitude, is reasonably well defined, we are led to conclude that even relatively sizable corrections to σ_e, if required, would not modify our finding that v_R decreases with temperature.

In Fig. 3, we show how a small change in the value of v_R results in a noticeable shift of the peak. The modification in v_R produces no discernible change in the average positron energy $E(t)$, and we see that the shift in the peak is immediately attributable, consistent with the slowing-down approximation, to the change in the time required for an "average" positron to reach an energy of E_R.

Finally, our calculations show that at zero electric field the sink-like and non-sink-like models give identical spectra.[22]

2. *Variation of electric field*

While experiments at different temperatures already provide a good deal of information about slow-positron interactions with low-temperature helium, considerably more insight may be gleaned from an examination of spectra measured at various electric field strengths. The broadening of the peak (until it disappears in the high-field limit) and decrease in Z_e with applied fields seem at first glance to be difficult to reconcile with the cluster model, since in that picture application of electric fields comparable to those considered here should have no effect on either of the parameters v_R and Z_R which characterize the clusters. Perhaps the most significant result of our calculation is that the changes in the positron velocity distribution induced by the field appear sufficient in themselves, *without any modification of the parameters in the cross sections*, to account for the observed electric field effects.

Monte Carlo calculations were performed of annihilation spectra at 5.5 °K in uniform electric fields of 0.0, 0.1, and 0.4 V cm^{-1} amagat^{-1}. The

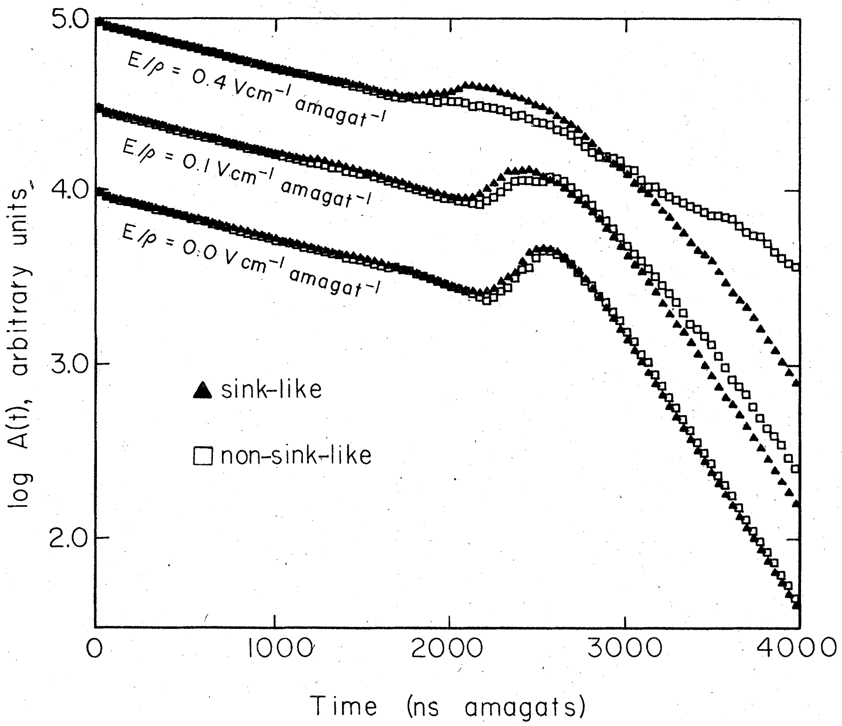

FIG. 4. Lifetime spectra calculated for slow positrons in high-density helium gas at 5.5°K in the presence of external electric fields. $E_R = 0.005$ eV, $Z_R = 18.2$.

cross sections employed were identical to those described above for the field-free calculations, and the modified Skullerud[21] method discussed in Sec. III was used to simulate the trajectories in the electric field. Both the sink-like and non-sink-like models were investigated.

A simple slowing-down analysis of the problem suggests that if λ_R and v_R are kept constant while the field is increased at constant temperature, then the peak should shift to somewhat longer time, while Z_e should decrease slightly. The acceleration of the field should delay the positrons' progress toward the threshold velocity v_R, thereby shifting the peak to longer time. The presence of the field will raise the equilibrium positron energy, thereby causing a decrease in the equilibrium annihilation rate.

As we see in Fig. 4, the calculations do show the expected and experimentally observed decrease in Z_e with increasing field. We also note the lowering and broadening of the peak in agreement with experiment. However, in contrast to the prediction of the slowing-down approximation, there is a small shift in the peak to *shorter* time. The magnitude of the shift is consistent with the lack of a significant shift reported by Deshpande.[9] To understand both the shift and the change in shape of the peak, we must consider an effect neglected by the slowing-down model, the increase in the width of the positron energy (or velocity) distribution with increasing electric field. Figure 5 shows this width as a function of time for positrons both with and without electric fields.

The slowing down approximation is quite successful at very low fields because the positron velocity distribution is sufficiently narrow that the behavior of a "typical" positron accurately characterizes the fate of the entire ensemble. When the distribution broadens, the approximation begins to break down. The acceleration of the electric field increases the average positron energy at any given instant, but it also enables some positrons with directions opposed or nearly opposed to the field to lose energy considerably faster than they could with no field present. The net result

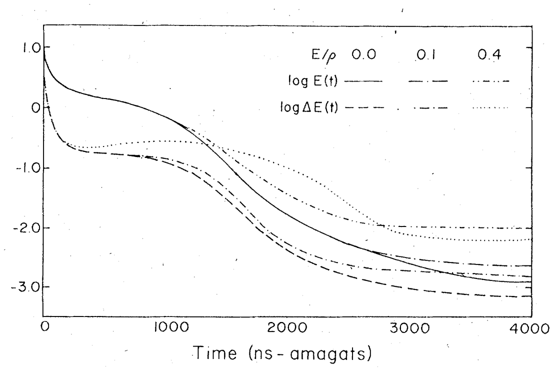

FIG. 5. Average energy $E(t)$ and width of energy distribution $\Delta E(t)$ for slow positrons in high-density helium gas at 5.5°K. All parameters as in Fig. 1.

of this broadening of the velocity distribution is to spread out the range of times at which positrons reach v_R, leading to an increase in the annihilation rate at times both before and after the field-free peak (see Fig. 4). This effect is observed as a broadening of the peak, and since the positrons which reach v_R earlier tend to cluster more than those which are delayed by the field, an apparent shift in the peak to shorter times is seen.

The effect of increasing electric field on the Z_e calculated in our models is somewhat surprising and potentially very revealing. One might expect that if λ_R were not changed, then the Z_e obtained in our calculations would vary slightly, if at all, from its zero-field value of $Z_R = \lambda_R / \pi r_0^2 c\rho$. This expectation must, of course, be fulfilled at sufficiently long times, since in that limit all the positrons will annihilate at velocities below v_R. However, as Fig. 4 shows, the times used in our calculations, which were chosen to roughly simulate experimental conditions, appear to lie sufficiently far from the long-time limit that increasing the field markedly affects the apparent[4] Z_e. This result is a reassuring one, since it is also what is observed experimentally. Thus we can, at least qualitatively, reproduce the experimental spectra in the presence of an external field *without changing the parameters from their field-free values.*

In Fig. 6, we present some experimental results as well as our calculated values of Z_e at various values of the applied electric field. While our calculations certainly reproduce the observed trend, the quantitative agreement is less satisfactory. However, obtaining a precise value of Z_e when both the calculated and experimental spectra are quite nonexponential in the tail region is a difficult task.[4] Also, the experimental data may be significantly affected by inhomogeneities in the applied fields.[9] The error bars on the experimental points probably represent a serious underestimate of the uncertainties in Z_e, since they are statistical only and do not take into account the large deviation of the experimental tail from a pure exponential.[9] The calculated error bars arise primarily from uncertainties associated with measuring the slope of the tail rather than from statistical considerations.

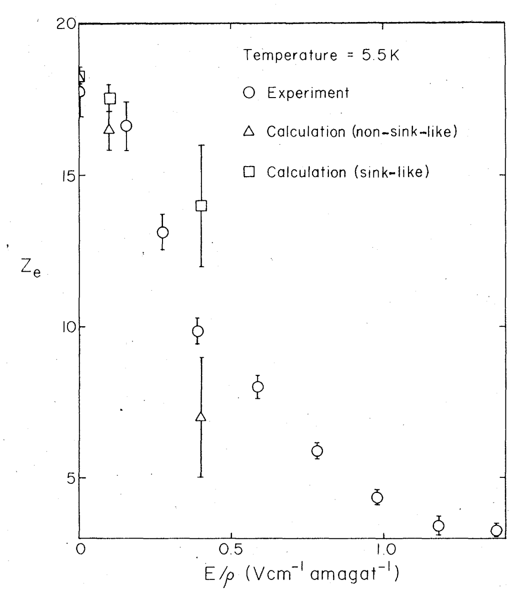

FIG. 6. Experimental (Ref. 9) and calculated values of Z_e for positrons in helium gas at 5.5 °K in external electric fields. All parameters as in Fig. 1.

In the non-sink-like model, Z_e is significantly more sensitive to the electric field strength than in the sink-like model. No choice can be made between the two models on the basis of their rather limited agreement with the experimental Z_e values. Since the calculations do predict significant differences between the two models, however, more accurate measurements, particularly at longer times where the problem of nonexponentiality would be less significant, should be well worthwhile.

Physically, the decrease in Z_e is still another effect of the increased width of the positron-velocity distribution as the field is increased. In a sense, both the lower value of Z_e and the nonexponential nature of the long-time section of the spectrum result from the overlap of the broadened peak with the previously distinct equilibrium decay region. The electric field has a greater effect in the non-sink-like model because it is able to accelerate positrons from velocities below v_R to velocities above threshold where the positrons are relatively "safe" from annihilation.

V. DISCUSSION

The present calculations clearly demonstrate the utility of the Monte Carlo approach in studying slow positrons in low-temperature, high-density helium gas, with or without external electric fields. The simple two-parameter model[16] employed in this study has enabled us to generate spectra in excellent agreement with those observed experimentally over a rather wide range of temperatures and applied fields. The behavior of the parameters is reassuringly consistent with the physical picture of cluster formation.[5] Whether the discrepancies that remain between theory and experiment derive primarily from inadequacies in our model or from inaccuracies in the data is unclear at this time. Certainly, the inhomogeneities in the external field discussed by Deshpande[9] are a potential source of error, and should be minimized in future experiments. Alternatively, if more homogeneous fields prove too difficult to obtain, the effects of inhomogeneities of a given form and magnitude could be simulated and studied using a slight modification of the methods employed here.

The model employed in the non-sink-like case is clearly oversimplified, especially at velocities below the threshold. Nevertheless, the success of the overall model as well as its ability to distinguish between sink-like and non-sink-like behavior are encouraging. A more stringent test of this or another model would require experimental data at a variety of temperatures and field strengths sufficiently accurate over the entire spectrum that one could meaningfully examine more than just two or three parameters. The detailed shape of the peak, the slope of the shoulder, and the deviations from pure exponential behavior in the tail, for example, should provide important information complementary to that derived from the location of the peak and the slope of the tail.

Other calculations of positron annihilation spectra of rare gases in electric fields[2,13,14,23-25] have focused on the high-temperature behavior and on the equilibrium decay rate. These calculations have all employed the diffusion equation. Aside from the difficulties involved in extracting the full spectrum from the diffusion equation approach, there is also some confusion about the exact form to be employed for the equation[9] when external fields are present. These problems arise from the directional averaging employed, which makes it possible to deal only with the magnitudes of $\vec{E}$ and $\vec{v}$. In our Monte Carlo calculation, as noted earlier in connection with the elastic scattering cross section, no such averaging is required and any anisotropies physically present are preserved. While our Monte Carlo study has not resolved the question of what values to use for the various coefficients in the diffusion equation, the results obtained here are independent of these quantities, since only the annihilation and scattering cross sections are required as input data.

We should note that when strong electric fields are present, considerably more positrons (often five to ten times as many) are required to obtain statistical accuracy comparable to that achieved in field-free Monte Carlo calculations. Although use of the Skullerud method[21] for dealing with the field makes some contribution to the increased variability of the results, the primary cause lies in the increased width of the positron-velocity distribution in the presence of an electric field. When this distribution is broad, a hundred or so swarms are insufficient to provide a representative sampling of the positrons in the ensemble. This effect will, unfortunately, make Monte Carlo investigations of positron spectra in extremely high fields rather expensive.

Our results indicate that the slowing-down approximation is a worthwhile one at high temperatures and/or at low electric fields. At low temperatures and high fields, where the width of the velocity distribution becomes significant, the approximation is no longer adequate, and detailed calculations or a more refined approximation which allows for the broadening of the distribution become necessary.

We hope that these calculations will stimulate further experimental and theoretical work not only on helium, but on other rare gases and more complex systems as well. The Monte Carlo method provides a reliable, straightforward means of testing different models in both the equilibrium and nonequilibrium regions. The peak in the low-temperature spectrum is not unique to helium,[26] and it would be most interesting to see how widespread such features are and whether they arise from one or from a variety of positron-scatterer interaction phenomena.

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$$\lambda_e = \left\langle -\frac{1}{N(t)} \frac{dN(t)}{dt} \right\rangle,$$

where $N(t)$ is the number of positrons remaining at time t, and the brackets signify an average (e.g., using the least-squares procedure described in paper I) over the tail of the spectrum. If the positrons have indeed reached equilibrium, then λ_e is the equilibrium decay rate. If not, as is generally the case in the experiments dealt with in this paper, then λ_e may be considered a phenomenological quantity which describes the average long-time behavior of the system.

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