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Effect of the Positron-Phonon Interaction on Positron Motion*

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We have made a calculation of the effect of the positron-phonon interaction on positron motion in simple cubic metals. We use a slightly modified jellium model to treat the positron-phonon interaction, and several approximations are introduced. Still, we feel confident that our calculations are qualitatively correct, and we conclude that phonons must play a role in determining positron motion in metals at low temperatures. In this region, phonon excitation provides an important additional mechanism for energy loss although it does not appear to contribute significantly to the effective positron mass.

I. INTRODUCTION

THE present status of the problem of positron thermalization in simple metals (i.e., Li, Na, K, Rb, Cs) is one of qualitative agreement between theory and experiment in support of the view that positrons generally annihilate in these metals at temperatures below room temperature before they reach equilibrium with their surroundings. Experimental work by Kim, Stewart, and Carbotte[1] and a complimentary calculation by Woll and Carbotte[2] provides much of the evidence on which this view is based. The purpose of the present work is to estimate the importance of the effect of positron-phonon interaction on the process of thermalization in comparison with the effect of positron-electron interaction. The former was neglected by Woll and Carbotte[2] after some consideration of the positron and phonon dispersion curves. These curves intersect at extremely low energy, typically about 3°K and it is therefore reasonable to assume that positron-phonon coupling will be negligible at least in the range of energy relevant to thermalization. However, early work of DeBenedetti *et al.*,[3] who showed that positrons would thermalize in Au at room temperature due to interactions with phonons alone, suggests that this assumption may not be justified. Further evidence supporting this view may be found by looking at the analogous case of the damping of electronic excitations by phonon emission where it is known that the damping is dominated[4] by the phonons in the low-energy region (below about $\frac{1}{2}$ eV), except for the lowest energies.

A straightforward "first-principles" calculation is presented. The positron-phonon coupling constant is calculated in Sec. II using a modified jellium model approximation which allows us to take some account of the exclusion by Coulomb repulsion of the positron from regions close to the ions. The formalism parallels the familiar formalism of the electron-phonon interaction since the interactions are quite similar. In Sec. III, the rate of energy loss of the positron is obtained from the imaginary part of the positron self-energy and the contribution to the positron effective mass of phonon self-energy corrections is shown to be small, in agreement with the results of Mikeska.[5] The energy loss rate due to electron-hole pair excitation is combined with the phonon contribution in Sec. IV and the results are given in Sec. II. Numerical calculations are carried out for Na only. Calculations for the other metals in the alkali series can readily be obtained in the same way. An outline of what happens at finite temperatures is given in Sec. VI. Results are discussed in Sec. VII and conclusions are presented. Two Appendixes are included to give further details of the evaluation of the positron-phonon matrix element and the positron effective mass.

II. POSITRON-PHONON INTERACTION

Positrons interact with the ions of a metallic crystal through a repulsive Coulomb potential screened by the conduction electrons. The interaction is basically the same as the electron-ion interaction except for the change in sign and the absence of exchange scattering with the core and screening electrons. Formulation of the positron-phonon interaction is therefore similar to the well-known formulation of the electron-phonon interaction. Thus, if $\mathbf{r}_i$ and $\mathbf{R}_l$ are the positions of the ith positron and the lth ion and $V(\mathbf{r}_i-\mathbf{R}_l)$ is the interaction between them (assumed to be spin-independent), the contribution to the total Hamiltonian is

$$H_{\text{pos-ion}}=\sum_i\sum_l V(\mathbf{r}_i-\mathbf{R}_l)=\sum_i W(\mathbf{r}_i),$$

where

$$W(\mathbf{r})=\sum_l V(\mathbf{r}-\mathbf{R}_l).$$

In second-quantized form, $H_{\text{pos-ion}}$ becomes

$$H_{\text{pos-ion}}=\sum_{\mathbf{q}}\sum_{\kappa}\sum_{\sigma}\langle\boldsymbol{\kappa}+\mathbf{q}|W|\boldsymbol{\kappa}\rangle c_{\kappa+q\sigma}{}^{\dagger}c_{\kappa\sigma},\qquad(1)$$

where $c^{\dagger}$, c are positron creation and destruction operators and the complete set of positron wave functions $|\boldsymbol{\kappa}\rangle$ are taken to be Bloch functions defined by

$$|\boldsymbol{\kappa}\rangle=(1/\Omega^{1/2})u_{\kappa}(\mathbf{r})e^{i\boldsymbol{\kappa}\cdot\mathbf{r}},$$

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[1] S. M. Kim, A. T. Stewart, and J. P. Carbotte, Phys. Rev. Letters **18**, 385 (1967).

[2] E. J. Woll, Jr., and J. P. Carbotte, Phys. Rev. **164**, 985 (1967).

[3] S. DeBenedetti, C. E. Cowan, W. R. Konneker, and H. Primakoff, Phys. Rev. **77**, 205 (1950).

[4] J. R. Schrieffer, *Theory of Superconductivity* (W. A. Benjamin, Inc., New York, 1964).

[5] H. J. Mikeska, Phys. Letters **24A**, 402 (1967).

where Ω is the volume of the crystal and $u_\kappa(\mathbf{r})$ has the periodicity of the lattice. Hence

$$\langle\boldsymbol{\kappa}+\mathbf{q}|W|\boldsymbol{\kappa}\rangle=\frac{1}{\Omega}\sum_l e^{-i\mathbf{q}\cdot\mathbf{R}_l}\int d\mathbf{r}e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{R}_l)}\times V(\mathbf{r}-\mathbf{R}_l)u_{\kappa+\mathbf{q}}^*(\mathbf{r})u_\kappa(\mathbf{r}).\quad(2)$$

If we let $\mathbf{x}=\mathbf{r}-\mathbf{R}_l$, it follows that

$$\langle\boldsymbol{\kappa}+\mathbf{q}|W|\boldsymbol{\kappa}\rangle=NS(\mathbf{q})M_{\kappa+\mathbf{q},\kappa},\quad(3)$$

where $S(\mathbf{q})$ is the structure factor defined by

$$S(\mathbf{q})=\frac{1}{N}\sum_l e^{-i\mathbf{q}\cdot\mathbf{R}_l},$$

and $M_{\kappa+\mathbf{q},\kappa}$ is the single-ion matrix element given by

$$M_{\kappa+\mathbf{q},\kappa}=\frac{1}{\Omega}\int e^{-i\mathbf{q}\cdot\mathbf{x}}u_{\kappa+\mathbf{q}}^*(\mathbf{x})u_\kappa(\mathbf{x})V(\mathbf{x})d\mathbf{x}.\quad(4)$$

N is the number of primitive cells in the crystal. For the metals, Li, Na, K, Rb, and Cs, there is one ion per primitive cell. The ion potential is well localized in the crystal so that the integral in Eq. (4) really extends only over one cell.

$S(\mathbf{q})$ may be expanded for small displacements $\mathbf{U}_l$ about the equilibrium lattice sites $\mathbf{R}_l^0$. To first order in the displacements,

$$S(\mathbf{q})=\frac{1}{N}\sum_l e^{-i\mathbf{q}\cdot\mathbf{R}_l^0}(1-i\mathbf{q}\cdot\mathbf{U}_l).\quad(5)$$

The first term leads to the static crystal field; the second leads to the positron-phonon interaction. Using Eqs. (1), (3), and (5), we can therefore express this interaction in the form

$$H_{\text{pos-ph}}=-i\sum_{\mathbf{q}}\sum_\kappa\sum_\sigma M_{\kappa+\mathbf{q},\kappa}\sum_l e^{-i\mathbf{q}\cdot\mathbf{R}_l^0}\mathbf{q}\cdot\mathbf{U}_l c_{\kappa+\mathbf{q}\sigma}^\dagger c_{\kappa\sigma}.$$

$\mathbf{U}_l$ can now be expressed in terms of the normal coordinates $Q(\mathbf{k},\lambda)$ through the relationship

$$\mathbf{U}_l=(MN)^{-1/2}\sum_{\mathbf{k}}\sum_\lambda Q(\mathbf{k},\lambda)\epsilon_\lambda(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{R}_l^0},$$

where the sum on $\mathbf{k}$ extends over the first Brillouin zone (FBZ) and M is the ion mass. Introducing the phonon creation and annihilation operators $a_{\mathbf{q}\lambda}^\dagger$ and $a_{\mathbf{q}\lambda}$ which are related to the normal coordinates through the relationship

$$Q(\mathbf{k},\lambda)=[2\omega_\lambda(\mathbf{k})]^{-1/2}(a_{-\mathbf{k}\lambda}^\dagger+a_{\mathbf{k}\lambda}),$$

and substituting for $\mathbf{U}_l$ and $Q(\mathbf{k},\lambda)$ in $H_{\text{pos-ph}}$ gives the familiar looking result

$$H_{\text{pos-ph}}=\sum_\kappa\sum_{\mathbf{q}}\sum_\sigma\sum_\lambda g_{\kappa+\mathbf{q},\kappa,\lambda}c_{\kappa+\mathbf{q}\sigma}^\dagger c_{\kappa\sigma}(a_{-\mathbf{q}\lambda}^\dagger+a_{\mathbf{q}\lambda}),$$

where the coupling constant is given by

$$g_{\kappa+\mathbf{q},\kappa,\lambda}=-i[\hbar N/2\omega_\lambda(\mathbf{q})M]^{1/2}\mathbf{q}\cdot\epsilon_\lambda(\mathbf{q})M_{\kappa+\mathbf{q},\kappa},\quad(6)$$

and $\omega_\lambda(\mathbf{q})$ and $\epsilon_\lambda(\mathbf{q})$ are the frequencies and polarization vectors of phonons with polarization λ.

Evaluation of the matrix element $M_{\kappa+\mathbf{q},\kappa}$ is carried out in Appendix A and is based on a slightly improved jellium approximation, using known positron wave functions calculated by Carbotte.[6] It is shown that, for Na,

$$M_{\kappa+\mathbf{q},\kappa}=\frac{1}{\Omega}\frac{4\pi e^2}{q^2}|u_0|^2\simeq\frac{1}{\Omega}\frac{4\pi e^2}{q^2}\frac{1}{\sqrt{2}},$$

i.e., the matrix element is the simple plane-wave matrix element multiplied by a numerical factor which is derived from the calculated positron wave functions. This factor is a measure of the exclusion by Coulomb repulsion of the positron from regions close to the ion cores. For two reasons, this approximate treatment of the matrix element is expected to be reasonably good. First, in the simple cubic metals considered here, for normal processes the coupling to transverse phonons is negligible because the polarization vector is very nearly perfectly normal to the propagation vector throughout the FBZ. Second, because the thermalization process is determined almost entirely by what happens below positron energies of about 0.1 eV, umklapp processes can be ignored since they are energetically impossible at these energies. Hence, the coupling constant simplifies to

$$g_q=-i[\hbar N/2\omega_\lambda(q)M]^{1/2}\frac{1}{\Omega}\frac{4\pi e^2}{q}|u_0|^2.\quad(7)$$

The screened coupling constant $\bar{g}_q$ is related to g_q by

$$\bar{g}_q=g_q/\epsilon(\mathbf{q},\omega),\quad(8)$$

where $\epsilon(\mathbf{q},\omega)$ is the dielectric function of the conduction electron gas. It has been shown by Carbotte and Arora[7] that the static, long-wavelength limit of the random-phase approximation (RPA) dielectric function is a good approximation when electron-hole pair excitation is the dominant thermalization mechanism. That this is so follows from the fact that the thermalization process is dominated by small momentum transfers and hence small energy transfers. We will assume that the same approximation holds good for thermalization due to phonon excitation because in the region of positron energy where the rates of energy loss due to phonon excitation and to electron-hole pair excitation become comparable, it can be shown that only momentum transfers $\overset{\sim}{<}\frac{1}{10}\lambda$ are allowable, where λ is the reciprocal of the Thomas-Fermi screening length. Hence,

$$\epsilon(\mathbf{q},\omega)\rightarrow\epsilon_{q\rightarrow0}^{\text{RPA}}(\mathbf{q},0)=1+\lambda^2/q^2\simeq\lambda^2/q^2,\quad(9)$$

where λ is related to the Fermi wave-vector by the

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[6] J. P. Carbotte, Ph.D. thesis, McGill University, 1964 (unpublished).

[7] J. P. Carbotte and H. L. Arora, Can. J. Phys. 45, 387 (1967).

equation

$$\lambda^2 = 4\kappa_F/\pi a_0,$$

where a_0 is the Bohr radius.

In the model we are using here, the (dressed) phonon frequencies $\omega(q)$ are given by

$$\omega(q) = (m/3M)^{1/2} v_F q = \sigma q, \tag{10}$$

where m is the electron mass, v_F the Fermi velocity, and σ the sound velocity. Using Eqs. (7)–(10), we find

$$\bar{g}_q \bar{g}_{-q} = (1/\Omega)|u_0|^4 \rho q, \tag{11}$$

where

$$\rho = 8\pi^2 e^4 \hbar n/\sigma M \lambda^4 \tag{12}$$

and $n = N/\Omega$, the density of conduction electrons.

III. POSITRON SELF-ENERGY

The full positron propagator contains a self-energy correction due to the interaction of the positron with phonons. The self-energy correction due to positron-electron interaction is omitted from the propagator here but the effect it produces on the rate of energy loss and the effective positron mass can be included later. Thus, within the Migdal[8] approximation, the self-energy of the positron $\Sigma(\boldsymbol{\kappa},\omega)$ is given by the lowest-order graph (Fig. 1).

The full positron and phonon propagators are defined in the momentum-energy representation by

$$G(\boldsymbol{\kappa},\omega) = 1/[\omega - E(\boldsymbol{\kappa}) - \Sigma(\boldsymbol{\kappa},\omega) + i\delta],$$
$$D(\mathbf{q},\epsilon) = 2\omega(q)/[\epsilon^2 - \omega^2(q) + i\delta],$$

where $\hbar$ has been dropped for convenience. $E(\boldsymbol{\kappa})$ is the positron dispersion relation in the noninteracting system.

Evaluating the self-energy graph according to the usual rules (given, for example, by Schrieffer[4]), we get

$$\begin{aligned}
-i\Sigma(\boldsymbol{\kappa},\omega)
&= \sum\nolimits_{\mathbf{q}} \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} iG(\boldsymbol{\kappa}+\mathbf{q},\, \omega-\epsilon) iD(-\mathbf{q},\, \epsilon) \bar{g}_q \bar{g}_{-q} (-i)^2 \\
&= \sum\nolimits_{\mathbf{q}} \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} \bar{g}_q \bar{g}_{-q} \\
&\quad \times \frac{1}{\omega - \epsilon - E(\boldsymbol{\kappa}+\mathbf{q}) - \Sigma(\boldsymbol{\kappa}+\mathbf{q},\, \omega-\epsilon) + i\delta} \\
&\quad \times \left(\frac{1}{\epsilon - \omega(q) + i\delta} - \frac{1}{\epsilon + \omega(q) - i\delta} \right)
\end{aligned} \tag{13}$$

on substituting for the propagators. Equation (13) is an integral equation for the self-energy. To simplify the problem we assume that the self-energy correction to the noninteracting dispersion relation $E(\boldsymbol{\kappa}+\mathbf{q})$ is small, so that

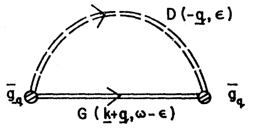

FIG. 1. Lowest-order positron self-energy correction due the positron-phonon interaction.

$$\Sigma(\boldsymbol{\kappa}+\mathbf{q},\, \omega-\epsilon)$$

may be dropped from the integrand in Eq. (13). This approximation can be restated by saying that the self-energy is determined almost entirely by the lowest-order diagram in which the dressed positron propagator is replaced by the bare positron propagator. This procedure has been shown by Migdal[8] to be quite reliable for the electron-phonon problem and we assume it is also applicable for the present work.

The intergral over ϵ can now be carried out by going to the complex ϵ plane and closing the contour in the lower half-plane. There is no contribution from the second part of the integrand and the result is

$$\Sigma(\boldsymbol{\kappa},\omega) = \sum\nolimits_{\mathbf{q}} \bar{g}_q \bar{g}_{-q} / [\omega - \omega(q) - E(\boldsymbol{\kappa}+\mathbf{q}) + i\delta].$$

Converting the summation on $\mathbf{q}$ to an integral according to the relation

$$\frac{1}{\Omega} \sum\nolimits_{\mathbf{q}} = \frac{1}{(2\pi)^3} \int d^3 q$$

and using the standard formula for factors appearing inside the integral

$$\frac{1}{x \pm i\epsilon} = P\frac{1}{x} \mp i\pi\delta(x),$$

we obtain the real and imaginary parts of $\sum(\boldsymbol{\kappa},\omega)$. Thus,

$$\sum\nolimits_R (\boldsymbol{\kappa},\omega) = \frac{\Omega}{8\pi^3} P \int \frac{d^3 q \bar{g}_q \bar{g}_{-q}}{\omega - \omega(q) - E(\boldsymbol{\kappa}+\mathbf{q})}, \tag{14}$$

$$\sum\nolimits_I (\boldsymbol{\kappa},\omega) = \frac{\Omega}{8\pi^3} \pi \times \int d^3 q \bar{g}_q \bar{g}_{-q} \delta[\omega - \omega(q) - E(\boldsymbol{\kappa}+\mathbf{q})], \tag{15}$$

where P denotes that the principal value of the integral is to be taken. Evaluation of $\Sigma_R(\boldsymbol{\kappa},\omega)$ shows that it leads to only a small correction to $E(\boldsymbol{\kappa})$ which can therefore be represented in terms of an effective positron mass. Details of this calculation are given in Appendix B where it is shown that the self-energy correction arising from positron-phonon interaction produces an increase in the positron mass of a few percent, in agreement with the results of Mikeska.[5] Throughout the subsequent calculations this correction will be neglected. The positron mass will be denoted by m^* and any deviation of m^* from m will be due entirely to positron-electron

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[8] A. B. Migdal, Zh. Eksperim. i Teor. Fiz. **34**, 1438 (1958) [English transl.: Soviet Phys.—JETP **7**, 996 (1958)].

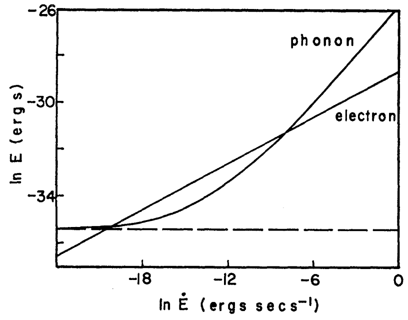

FIG. 2. Relationship between the two components of the total energy loss rate [see Eq. (18)] and the positron energy. A logarithmic plot shows both curves to be linear at high energy. At lower values of E the phonon component of the rate decreases more rapidly to zero as the positron drops to an energy corresponding to a few degrees absolute. At this point the "classical" speed of the positron is equal to the speed of sound.

effects. Hence we can replace ω by $\kappa^2/2m^*$ in Eq. (15) to a good approximation. Σ_I is directly proportional to the damping rate of the positron by phonons and hence is closely related to the thermalization rate of the positron.

IV. POSITRON ENERGY LOSS RATE

Assuming that the positron decays from one well-defined momentum state into another such state, the probability for such a transition with momentum transfer $\hbar\mathbf{q}$ is related to the imaginary part of the self-energy by the equation

$$1/\tau = -2\Sigma_I/\hbar.$$

The same result can be obtained directly from the Fermi Golden Rule for transition probability. The rate at which the positron loses energy is simply the transition probability (or damping rate) times the energy transfer associated with the momentum transfer $\hbar\mathbf{q}$. This energy is just $\hbar\sigma q$, the energy of the created phonon. It must be included inside the integrand of Eq. (15) and hence the rate of energy loss $\dot{E}(\boldsymbol{\kappa})$ is given by

$$\dot{E}(\boldsymbol{\kappa}) = \frac{\Omega}{4\pi^2\hbar}\int d^3q\, \bar{g}_q\bar{g}_{-q}\hbar\sigma q \times\delta\left[\hbar\omega-\hbar\sigma q-\frac{\hbar^2}{2m^*}(\boldsymbol{\kappa}+\mathbf{q})^2\right], \quad (16)$$

where $\hbar$ has been restored. Defining the constant β by

$$\beta = 2m^*\sigma/\hbar$$

and letting μ be the cosine of the angle between $\boldsymbol{\kappa}$ and $\mathbf{q}$, we obtain

$$\dot{E}(\kappa) = -\frac{m^*\Omega\sigma}{2\pi\hbar^2\kappa}\int_1^{-1}\int_a^b q^2dq\, d\mu\, \bar{g}_q\bar{g}_{-q}\delta\left(\mu+\frac{q+\beta}{2\kappa}\right)$$

using the simplification discussed earlier that $\omega=\kappa^2/2m^*$. The limits on the q integral a and b are determined by the integration over μ. Cylindrical symmetry about the direction of $\mathbf{q}$ is assumed. Substituting from Eq. (11), we find

$$\dot{E}(\kappa) = -\frac{\rho m^*|u_0|^4\sigma}{2\pi\hbar^2\kappa}\int_1^{-1}\int_a^b q^3dq\, d\mu\, \delta\left(\mu+\frac{q+\beta}{2\kappa}\right).$$

On integrating over μ, it follows that $\dot{E}(\kappa)=0$ except for values of q satisfying the condition

$$1 \geqslant -(q+\beta)/2\kappa \geqslant -1,$$

in which case

$$\dot{E}(\kappa) = -(2\rho m^*\sigma|u_0|^4\kappa^3/\pi\hbar^2)(1-\beta/2\kappa)^4. \quad (17)$$

From the above conditions on q and the requirement that $q\geqslant 0$, the values of a and b are found to be 0 and $2\kappa-\beta$, respectively.

Two comments, may be made on Eq. (17). First, $\dot{E}(\kappa)$ is proportional to $E^{3/2}$ at high energy (i.e., $\kappa\gg\beta$). Comparing this to the E^3 dependence of $\dot{E}$ due to electron-hole pair excitation, it follows that the latter mechanism will dominate the thermalization process in the early stages and will become less important as the positron energy drops. The crucial question is: At what energy does the phonon contribution become non-negligible? An estimate of this energy for sodium is given in Sec. V. Second, it can be seen that $\dot{E}(\kappa)\to 0$ as $2\kappa\to\beta$. This reflects the impossibility of conserving momentum and energy in the phonon creation process when the positron energy becomes very small. On a simple classical picture, $\dot{E}(\kappa)$ tends to zero when the positron velocity approaches the speed of sound.

Equation (17) gives the rate of energy loss of the positron due to phonon excitation. In order to determine whether this rate is large enough to materially change the accepted thermalization times in the alkali metals, it must be combined with the energy loss rate due to electron-hole pair excitation and new thermalization times calculated. Thus, expressing Eq. (17) in terms of the positron energy E, the total rate of energy loss can be written

$$\dot{E} = \dot{E}_{\rm el}+\dot{E}_{\rm ph} = -[FE^3+HE^{3/2}(1-G/E^{1/2})^4], \quad (18)$$

where the constants are given by

$$F = (8/105)(\pi m^*/2m\hbar E_F),$$
$$G = \tfrac{1}{2}\beta(\hbar^2/2m^*)^{1/2},$$
$$H = (2\pi^3e^4nm^{*2}a_0^2|u_0|^4/\hbar^3\kappa_F^2M)(2m^*/\hbar^2)^{1/2}.$$

The first term in Eq. (18) is the Carbotte-Arora[7] result for the loss rate due to electron-hole pair excitation as given by Woll and Carbotte[2] [Eq. (B2) of that paper]. The constants F, G, and H can be evaluated for each metal in the series. $|u_0|^4$ is taken to be 0.5 (see Appendix A) for sodium. Equation (18) can then be integrated numerically.

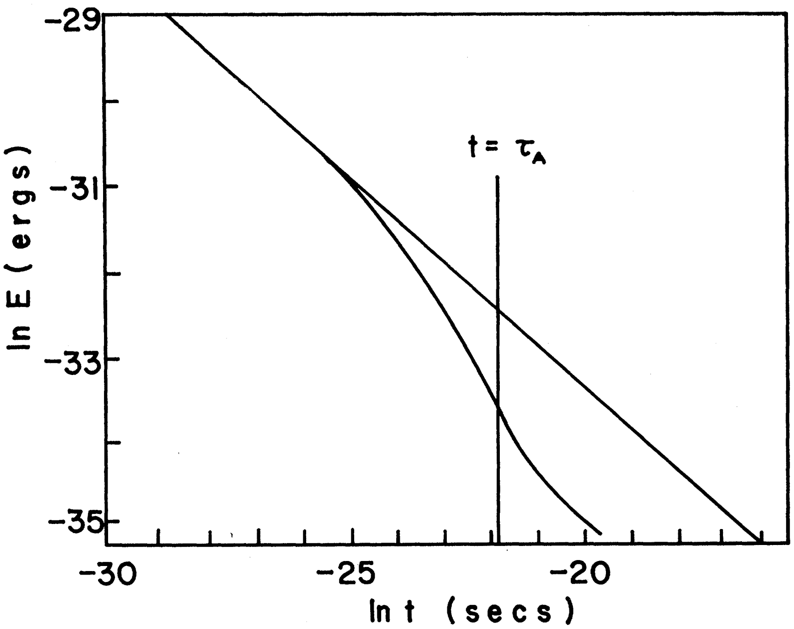

FIG. 3. Positron energy as a function of time using logarithmic scales. The curve is linear at high energy (i.e., early times) showing that the electron component dominates. As the phonon component becomes more important the energy drops below that predicted by considering only the electron component of the total rate. Since the annihilation time τ_A falls on the axis in the region where the deviation is appreciable, a significantly different result is obtained from that given by earlier theories for the minimum positron energy on annihilation.

V. RESULTS

A rough measure of the relative importance of the electron and phonon components of Eq. (18) can be obtained by plotting the logarithms of the respective contributions to the total rate of energy loss against the logarithm of the positron energy (Fig. 2). The electron component and the phonon component at high energy are linear. At lower energy the phonon component decreases more rapidly as the $(1-G/E^{1/2})^4$ factor becomes important. The energy E_c, at the crossover point in Fig. 2 gives us some idea of the thermalizing capabilities of the electrons and phonons. This crossover is a characteristic of the different energy dependence of each of the two components of the total rate of energy loss. For sodium, E_c is about $190k_B$ erg, taking m^* equal to m. It can be found from the results presented in Fig. 3 that the positron reaches this energy after a time of 0.23×10^{-10} sec. This corresponds to roughly 1/14 of the positron lifetime against annihilation τ_A showing that the positron would appear to have plenty of time to couple effectively to the phonon system before annihilating. Figure 3 shows the positron energy as a function of time. The curve is computed by numerical integration of Eq. (18) subject to certain initial conditions. It was mentioned earlier in Sec. II that umklapp processes could be neglected in calculations of thermalization times. This follows from Eq. (18) since, neglecting the phonon contribution, the equation can be easily integrated to give

$$t=1/2FE^2,$$

where it has been assumed that the positron enters the metal with infinite energy at time $t=0$. For Na, $F\simeq4.6\times10^{37}$ erg^{-2} sec^{-1} and therefore for the positron to fall to an energy of the order of 1 eV takes about 4×10^{-15} sec. Since this time is very much less than τ_A it follows that we can safely take the initial positron energy to be about $\frac{1}{4}E_F$ in calculations of thermalization times. Thus the initial positron wave vector is taken to be about $\frac{1}{2}\kappa_F\simeq\frac{1}{2}q_D\simeq\frac{1}{2}q_{BZ}$, where κ_F, q_D, and q_{BZ} are characteristic dimensions of the Fermi sphere, the Debye sphere, and FBZ, respectively. The neglect of umklapp processes is therefore justified and Eq. (18) may be integrated numerically subject to the above condition.

It can be seen from Fig. 3 that the positron energy falls well below the value expected on the basis of zero positron-phonon coupling (straight line). Whether this will affect the predicted energy on annihilation E_A depends on where τ_A falls on the time axis. For Na we find that $E_A=18°\text{K}\times k_B$ compared to $59°\text{K}\times k_B$ for the Carbotte-Arora[7] case where there is no coupling to the phonons.

The figures given above are for $m^*=m$. On using $m^*=2m$, we obtain more pronounced phonon effects. For example, E_c is doubled to $380°\text{K}\times k_B$.

VI. EXTENSION TO FINITE TEMPERATURES

At finite temperatures the net rate of energy loss by the positron is reduced by collisions in which phonons are absorbed and which therefore lead to an increase in positron energy. A similar statement can be made in the case of the interaction with the electron gas and this feature has been included in the calculation of Woll and Carbotte.[2] In order to include "scattering in" terms where phonons of wave vector $\mathbf{q}$ are absorbed by the positron, Eq. (16) must be modified by introducing the appropriate distribution functions for the phonons. Thus,

$$\dot{E}(\boldsymbol{\kappa}) = \frac{\Omega}{4\pi^2\hbar}\left[\int d^3q\, \bar{g}_q\bar{g}_{-q}\hbar\sigma q[n(q)+1] \times\delta\left(\hbar\omega-\hbar\sigma q - \frac{\hbar^2}{2m^*}(\boldsymbol{\kappa}+\mathbf{q})^2\right) - \int d^3q\bar{g}_q\bar{g}_{-q}\hbar\sigma q \times[n(q)]\delta\left(\hbar\omega+\hbar\sigma q - \frac{\hbar^2}{2m^*}(\boldsymbol{\kappa}+\mathbf{q})^2\right)\right],$$

where $n(q)$ is the Bose-Einstein function given by

$$n(q)=[\exp(\hbar\sigma q/k_BT)-1]^{-1}.$$

Evaluating the integrals over the angles leads to the result

$$\dot{E}(\kappa)=-(2\rho m^*\sigma u_0{}^4/\pi\hbar^2)\kappa^3R(\kappa,T)\,, \tag{19}$$

where

$$R(\kappa,T) = \frac{1}{4\kappa^4}\left(\int_0^{2\kappa-\beta} q^3dq - \int_{2\kappa-\beta}^{2\kappa+\beta} q^3n(q)dq\right). \tag{20}$$

On comparing Eqs. (19) and (20) with Eq. (17), it can be seen that the first integral of $R(\kappa,T)$ gives the zero-temperature result while the second integral can be regarded as a finite temperature correction. $R(\kappa,T)$ can be evaluated by numerical integration. It is then found that $\dot{E}(\kappa)$ decreases linearly with increasing sample temperature T for sample temperatures above about 50°K. At lower sample temperatures $\dot{E}(\kappa)$ is a relatively insensitive function of T.

It is also found that $\dot{E}(\kappa)\rightarrow 0$ as $E\rightarrow 2k_BT$ and therefore we would have to conclude that the positron was "thermalized" (i.e., in equilibrium with the phonon gas) at an energy of $2k_BT$ and not $\frac{3}{2}k_BT$. This surprising result is a consequence of using the simple "δ-function" distribution for the positron instead of the more accurate Maxwell-Boltzman distribution. This result can be obtained directly from Eq. (19) by setting $R(\kappa,T)$ equal to zero and evaluating the integrals approximately since $\kappa\gg\beta$, except for extremely low positron energies of the order of a few degrees.

The temperature-dependent rate of energy loss can be combined with the contribution from electron-hole pair excitation as before to obtain E-versus-t curves for various sample temperatures. Unfortunately, for the reason mentioned above, we cannot regard these curves as quantitatively reliable. However, we do find that our simple model predicts that the greater the effective positron mass m^*, the shorter will be the thermalization time. In order to give reliable numerical estimates of these times and of minimum positron energies on annihilation, in samples at nonzero temperatures, a full finite-temperature calculation of the Woll-Carbotte[2] type will have to be done including both the effects of electrons and phonons.

VII. DISCUSSION

Some mention has already been made of the work of Woll and Carbotte[2] on positron thermalization in an electron gas at finite temperatures. Their approach takes proper account of the statistical nature of the energy-loss process. The simple picture used by Carbotte and Arora[7] and by the present authors in which the positron decays successively through a series of well-defined states is replaced by one which allows the positron to decay into a distribution of final states with probability given by the Fermi Golden Rule. The results obtained by Woll and Carbotte[2] agree quite well with those of Carbotte and Arora[7] and give qualitative agreement with the experimental results of Kim, Stewart, and Carbotte.[1] However the theory gives a thermalization rate greater than that which is deduced from experiment. That is, the predicted minimum positron energy is somewhat lower than the experimental value. The results presented here give an even lower minimum positron energy in Na at zero sample temperature and hence lead to an even greater disagreement with experiment. However, although the present model predicts that positrons will thermalize at much lower temperatures than those at which Kim, Stewart, and Carbotte[1] have obtained evidence of nonthermalization, it only permits a reliable estimate of the minimum positron energy on annihilation in a sample at zero temperature. Any attempt to obtain by computation curves similar to those of Kim, Stewart, and Carbotte[1] would involve a full Woll-Carbotte-type[2] calculation.

Such a calculation would require considerable effort and it is unlikely that the results would lead to closer agreement with experiment that those given here. Also, such an effort would not be justified without refining the present model used for the positron-ion interaction as well as our use of the unperturbed propagator in the lowest-order graph.

However, because of the strong energy dependence of the coupling of the positrons to the phonons, it may be that some structure would show up in the low-temperature region. In any case further experimental work of greater accuracy and detail would be very useful at this point. It could provide the necessary stimulus to remove some of the approximations we have made and to obtain more accurate estimates of the role of phonons in positron thermalization.

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APPENDIX A

The evaluation of the matrix element $M_{\kappa+\mathbf{q},\kappa}$ given by Eq. (4) is simplified by noting that the functions $|u_{\kappa+\mathbf{q}}^*(\mathbf{x})|$ and $|u_\kappa(\mathbf{x})|$ can be replaced to a good approximation by $|u_0(\mathbf{x})|$. Since $u_0(\mathbf{x})$ has the periodicity of the lattice, it can be expanded in terms of the reciprocal-lattice vectors **G**. Hence,

$$u_0(\mathbf{x})=\sum_{\mathbf{G}} V_G \exp(i\mathbf{G}\cdot\mathbf{x}). \tag{A1}$$

Similarly, the ionic potential $V(\mathbf{x})$ can be expanded in a Fourier series:

$$V(\mathbf{x})=\sum_{\mathbf{q}'} V(\mathbf{q}') \exp(i\mathbf{q}'\cdot\mathbf{x}).$$

Substituting into Eq. (4) we obtain

$$\begin{aligned} M_{\kappa+\mathbf{q},\kappa} &= \frac{1}{\Omega}\sum_{\mathbf{q}'}\sum_{\mathbf{G}}\sum_{\mathbf{G}'}\int d\mathbf{x}\, V_G V_{G'} V(\mathbf{q}') \\ &\qquad\times\exp[i(\mathbf{G}-\mathbf{G}'+\mathbf{q}'-\mathbf{q})\cdot\mathbf{x}] \\ &=\sum_{\mathbf{G}}\sum_{\mathbf{G}'} V_G V_{G'} V(\mathbf{G}'-\mathbf{G}+\mathbf{q}). \end{aligned} \tag{A2}$$

The Fourier coefficients V_G appearing in Eq. (A1) have been calculated by Carbotte.[6] In order to carry out the summations in Eq. (A2) it is convenient to relabel the coefficients so that they indicate the position of each site in the reciprocal lattice with respect to the origin. Thus the matrix element can be expressed by

$$M_{\kappa+\mathbf{q},\kappa}=\sum_{i=0}^{N-1} V_i^2 V(\mathbf{q})+\sum_{i=0}^{N-1}\sum_{j=0,\ j\neq i}^{N-1} V_i V_j V(\mathbf{G}_j-\mathbf{G}_i+\mathbf{q}),$$

where V_0 is the coefficient referring to the origin and the remaining $N-1$ values refer to each of the other $N-1$ sites in the reciprocal lattice. For the metals under consideration here, the reciprocal lattice is fcc. There are therefore 12 nearest neighbors and six next nearest neighbors. Since the Fourier components of the potential are inversely proportional to $(|\mathbf{G}_j-\mathbf{G}_i+\mathbf{q}|^2+\lambda^2)$ and the coefficients V_G get very small after the first ($V_0=0.98620$), we can hope for some convergence in the summations. By including only nearest neighbors, for which

$$V_i(i=1,\ldots,12)=-0.04394,$$

it turns out that the long wavelength limit of the matrix element is 0.71 $V(\mathbf{q})$, where $V(q)$ is the plane-wave matrix element given by $(4\pi e^2/\Omega q^2)$. Including also the next nearest neighbors, for which

$$V_i(i=13,\ldots,18)=-0.01463,$$

the result is 0.69 $V(\mathbf{q})$. This reduction of the interaction between the positron and the ion cores is due to the reduced probability (arising from Coulomb repulsion) of finding the positron close to the ions. Since the rate of energy loss depends on the square of the matrix element, i.e., on $|u_0|^4$, it follows that the rate is reduced by a factor of 2 due to the exclusion of the positron from the regions close to the ions.

APPENDIX B

From Eq. (14) it follows that the real part of the positron self-energy can be written

$$\sum\nolimits_R(\boldsymbol{\kappa},\omega) = \frac{\Omega}{8\pi^3}\frac{2m^*}{\hbar^2}P\int d^3q\, \bar{g}_q\bar{g}_{-q}\Big/ \left(\frac{2m^*\omega}{\hbar}-\beta q-(\boldsymbol{\kappa}+\mathbf{q})^2\right).$$

Substituting from Eq. (11) and approximating $\hbar\omega$ by $\hbar^2\kappa^2/2m^*$,

$$\sum\nolimits_R(\boldsymbol{\kappa},\kappa^2) = -\frac{\rho m^* u_0^4}{2\pi^2\hbar^2}P\int\int\frac{q^2dq\, d\mu}{2\kappa\mu+q+\beta}.$$

The limits on the q integration are properly 0 and ∞, since $\sum_R(\kappa,\omega)$ is determined by virtual phonon processes which therefore include umklapp processes. Hence the integrand should be modified at the outset to take account of the umklapp processes. However, it turns out that the integral is insensitive to the upper limit and to the accuracy of the present calculation it is sufficient to replace the upper limit by q_D. The calculation of the integrals is straightforward and $\sum_R(\boldsymbol{\kappa},\kappa^2)$ is a smooth function of κ. The effective mass of the positron due to phonon interactions m_{ph}^* is obtained by solving the equation

$$\kappa^2-\omega-[\sum\nolimits_R(\boldsymbol{\kappa},\kappa^2)-\sum\nolimits_R(0,0)]=0$$

for ω and setting

$$\omega=\kappa^2/m_{ph}^*.$$

It is found that m_{ph}^* increases as κ decreases, reaching a maximum of about $1.03m^*$ in Na before decreasing as κ tends to zero.

Two checks have been made on the reliability of the first-order approximation $\omega=\kappa^2$. First, the equation

$$\kappa^2-\omega-[\sum\nolimits_R(\boldsymbol{\kappa},\omega)-\sum\nolimits_R(0,0)]=0$$

was solved numerically to compute the real dispersion relation for the positron. The result was not significantly different from the first order approximation. Second, a power-series-expansion method was used at small energies. Again, the effective mass was small.

However, the approximation $\omega=\kappa^2$ is bound to be bad near the region where the phonon and free-positron dispersion curves interact. These difficulties are well known; analogous situations arise in several branches of physics. Fortunately, the crossover point in this case lies so low in energy (only 2 or 3 deg above absolute zero) that the strong perturbations it produces in the dispersion curve produces a negligible effect on positron thermalization except, possibly, in samples at extremely low temperatures (<3°K).