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PHYSICAL REVIEW B VOLUME 3, NUMBER 5 1 MARCH 1971

Temperature Dependence of the Positron-Annihilation Angular Correlation in Metals*

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The thermal smearing of the positron-annihilation-angular-correlation curves is studied. In the case where the medium is a homogeneous interacting electron gas in thermal equilibrium, the analysis applied by Stewart and co-workers to the thermal smearing is shown to correctly give the effective mass. In conjuction with previous calculations of the effective mass, our results indicate that the observed thermal smearing cannot be explained as mainly caused by electron-gas effects. It is shown how the model can be modified to take into account the positron-phonon interaction. This reduces the discrepancy between theory and experiment, but not sufficiently to account fully for the experimental data. It is argued that new experiments are needed before one can decide whether it is necessary to consider new mechanisms in order to explain the effect. A convenient formalism is presented, which allows one to calculate all positron quantities at moderate nonzero temperatures within a given approximation scheme. The "ladder" approximation is used to illustrate the argument and to estimate correction terms.

I. INTRODUCTION

The temperature dependence of the 2γ angular correlation from positrons annihilating in alkali metals has been studied experimentally by Stewart and co-workers.[1,2] Employing a model described in detail by Kim,[2] they used their data to determine the ratio m^* of the effective and bare masses, and found the values 1.8 ± 0.3, 1.8 ± 0.2, 2.1 ± 0.3, 2.3 ± 0.3, respectively in Li, Na, K, and Rb. Calculations of the electron-positron,[3,4] positron-phonon,[5,6] and, in the case of Na, the band effective mass [2,7] all tend, however, to give values of m^* close to unity. This discrepancy makes it desirable to reexamine whether the experiment actually can be expected to give the positron effective mass.

The main purpose of the present paper is to demonstrate that, in the idealized case of a thermalized positron annihilating at moderate temperatures in an interacting electron gas, the above-mentioned

data analysis would indeed correctly give the effective mass. This is so provided allowance is made (as was done by Kim[2]) for the deviation of the zero-temperature angular-correlation curves from free-electron parabolas. If only electron-gas effects are taken into account the discrepancy between the observed and calculated thermal smearing persists. This leads us to believe that other effects need to be considered in order to account for the data.

Because of the smallness of the thermal effects, the reported measurements were carried out over a wide temperature region. The most significant experimental points were those taken near the melting point of the metal under study. For certain metals there is a rather dramatic change in the mean lifetime in this temperature region[8] due to trapping of positrons at vacancy sites.[9] This change is associated with a marked change in the angular correlation.[10] Recent measurements in the alkali metals indicate, however, no significant change in the positron lifetime before melting.[11,12] This may mean that the vacancy potential is too weak to trap positrons. We are not convinced that the available evidence completely rules out vacancy trapping. If trapping does occur the interpretation of the experiments would, of course, be strongly affected.

We mentioned that the positron-phonon interaction has been found to contribute negligibly to the positron effective mass. It has been pointed out, however, by Mikeska,[6] that thermal phonons significantly contribute to the imaginary part of the positron self-energy in a way which causes a non-Boltzmann-like momentum distribution for the positron quasiparticles. As will be seen, one can neglect this effect in the electron-gas case. When modified to take into account the electron-positron interaction, in a manner which will be described here, the Mikeska model gives rise to an increase in the "apparent" effective mass. The interactions with the phonons will also contribute to the high-momentum tail in the angular correlation. This contribution will, however, be swamped by core annihilation and one cannot expect to see the effect.

A crucial factor in the theory is that, for kinematical reasons, the thermal variation in the electron momentum distribution should be insignificant, in the interesting temperature region, compared to the momentum resolution of the angular-correlation technique.[1,2] Neglecting thermal effects on the electron momentum distribution we find, in Sec. II, sufficient conditions on the real and imaginary parts of the positron self-energy for the validity of the relationship between the thermal smearing and the effective mass assumed by Kim.[2] In Sec. III we show that in the electron-gas case these conditions appear to be well satisfied. For this purpose we have developed a convenient formalism which allows us to discuss all relevant quantities in the electron-positron system within the same approximation scheme. This enables us to estimate the effect of possible correction terms by using a model, the "ladder approximation," which is relatively crude, but which has been found to give reasonable results. One of the assumptions is not valid, when the positron-phonon interaction is taken into account, and we indicate how the fundamental formulas should be modified in this case. Our formal starting point is temperature-dependent many-body perturbation theory as adapted to the positron problem by Majumdar,[13] who, like Mikeska,[6] based his effective-mass formalism on the independent-particle approximation.

In assuming constant electron density as the temperature varies we ignore thermal expansion. The thermal expansion of the alkali metals is not small in the interesting temperature region, but the numerical method used in Refs. 1 and 2 automatically compensates for it.

II. THERMAL SMEARING AND EFFECTIVE MASS

Angular-correlation measurements performed with the parallel-slit geometry give the relative probability for one component of the c.m. momentum $\vec{K}$ of the annihilating pair to have a given value. This means that one measures something proportional to

$$\langle P(K_z)\rangle = \int_{-\infty}^{\infty} dK_x \int_{-\infty}^{\infty} dK_y\, E(\vec{K}). \tag{1}$$

$E(\vec{K})$, the "enhancement function," is the expectation value of the operator

$$P(\vec{K}) = \tfrac{1}{2} \sum_{\vec{p},\vec{p}',s} b_{\vec{p}}^{\dagger} d_{\vec{K}-\vec{p},s}^{\dagger}\, d_{\vec{K}-\vec{p}',s}\, b_{\vec{p}'}. \tag{2}$$

Here $d_{\vec{K},s'}^{\dagger}, b_{\vec{p}}^{\dagger}$ are, respectively, electron- and positron-creation operators in momentum space. For notational convenience we have suppressed the positron spin index. We have[14] for N^+ noninteracting positrons in thermal equilibrium with a noninteracting electron gas

$$E_0(\vec{K}) = (1/N^+) \textstyle\sum_{\vec{q}} g^-(q^2) f^-((\vec{K}-\vec{q})^2). \tag{3}$$

We can, in the limit of low density N^+/V, use in (3) a positron momentum distribution

$$g^-(q^2) \sim (8N^+/3NT^{3/2}\pi^{1/2}) e^{-q^2/T}. \tag{4}$$

The corresponding electron distribution can, for sufficiently low temperatures, be written as

$$f^-(z) \sim \eta(1-z) + \theta(z-1)\, e^{-|1-z|/T}, \tag{5}$$

where $z = |\vec{K}-\vec{q}|^2$ and

$$\begin{aligned} \eta(z) &= 1 \quad (z>0) \\ &= 0 \quad (z<0), \\ \theta(z) &= 1 \quad (z>0) \\ &= -1 \quad (z<0). \end{aligned} \tag{6}$$

At moderate temperatures (3) deviates from zero-temperature behavior for K values close to the Fermi surface. We write

$$K = 1 + \Delta. \tag{7}$$

Since for sufficiently small values of Δ we have[1,2]

$$|(1+\Delta)^2 - 1| \gg \Delta^2, \tag{8}$$

the *deviation* from $T=0$ behavior in (3) at moderate temperatures comes only from (4) and not from (5). We will in what follows use zero-temperature electron-distribution functions and only take into account the temperature dependence of the positron functions. This gives in the noninteracting case

$$E_0(\vec{K}) = (\pi T)^{-3/2} \int d^3q\, \eta(1 - |\vec{K} - \vec{q}|)\, e^{-q^2/T}. \tag{9}$$

It is easy to see by evaluating and comparing (3) and (9) that, at metallic densities, the thermal effects in (5) have a negligible influence on (3) even at temperatures as high as $T = 400\,^\circ$K, which is the maximum temperature of interest to us.

Let $\tilde{E}(\vec{K})$ be the $T=0$ enhancement function for the interacting system. Kim[2] *assumes*

$$E(\vec{K}) = (\pi m^* T)^{-3/2} \int d^3q\, \tilde{E}(\vec{K} - \vec{q})\, e^{-q^2/m^*T}. \tag{10}$$

We wish to check the validity of (10) by evaluating $E(\vec{K})$ formally and finding out what kind of assumptions are needed in order to obtain the equation. Adding a term $\lambda P(\vec{K})$ to the total Hamiltonian gives

$$E(\vec{K}) = \frac{1}{N^+} \frac{\partial \Omega}{\partial \lambda}\bigg|_{\lambda=0}, \tag{11}$$

where Ω is the grand thermodynamical potential. In perturbation theory this quantity is the sum over all linked vacuum-to-vacuum diagrams. These may contain zero, one, two, etc., positron loops. Only diagrams that contain positron lines contribute to the derivative in (11). In the physical limit of low positron density, only those diagrams contribute which contain one positron loop. This loop may have any number of self-energy insertions attached to it (see Fig. 1).

The free-positron thermodynamical propagator has the Fourier series

$$G_0(\vec{q}, t) = T \sum_n (z_n - q^2)^{-1} e^{z_n t}, \tag{12}$$

where $z_n = (2n+1) i\pi T + \mu_T$, $n = 0, \pm 1, \pm 2$, etc., and

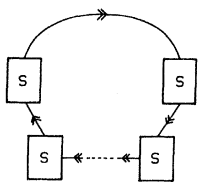

FIG. 1. Positron contribution to the grand potential is given by the sum of all linked vacuum-to-vacuum diagrams made up of one closed positron loop into which is inserted any number of proper self-energy insertions S. Lines with double arrows represent free-positron propagators.

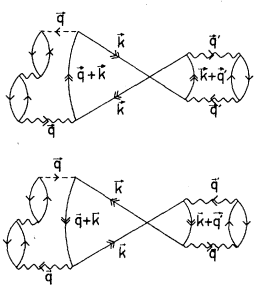

FIG. 2. (a) Typical diagram containing two proper self-energy insertions to a positron-hole line. The single arrow on a line indicates the free-electron propagator. Wavy lines represent the electron-electron or the electron-positron interaction, while the dotted line means a "rooted vertex." (b) Diagram with more than one hole line and nonrepeated hole-momentum label.

μ_T is the positron chemical potential which gives rise to an equilibrium positron concentration N^+/N. We write

$$\mu_T = \mu_0 + \mu, \quad y_n = z_n - \mu, \tag{13}$$

where μ is the energy one must contribute to the system per positron added to it. We call[13] a vertex "rooted" if it arises from the term $\lambda P(\vec{K})$ in the Hamiltonian. Let[15] $\tilde{S}(\vec{q}, \vec{K}, y_n)$ be the Fourier coefficient for the sum of all proper self-energy insertions to a positron line with momentum $\vec{q}$, and let $S(\vec{q}, \vec{K}, y_n)$ be the sum of all such self-energy insertions which do not contain any positron-hole lines. Clearly the difference between these two quantities is proportional to the positron density. We find from arguments similar to those of Luttinger and Ward[16]

$$\Omega - \Omega_0 = \sum_{l=0}^{\infty} \frac{T}{l} \sum_{\vec{g}} \sum_{n=-\infty} e^{z_n 0+} \left[\frac{S(\vec{q}, \vec{K}, y_n)}{z_n - q^2}\right]^l, \tag{14}$$

where Ω_0 is the electron contribution to the grand potential. The symmetry factor l is the number of times each contraction is included when all diagrams with l self-energy insertions are summed over. Note that it is $S(\vec{q}, \vec{K}, y_n)$ and not the complete self-energy $\tilde{S}(\vec{q}, \vec{K}, y_n)$ which enters in (14). The reason is that otherwise a diagram such as Fig. 2(a) would be considered both as having one proper self-energy insertion to the positron line labeled by $\vec{q}+\vec{k}$ and as having two proper insertions to the line labeled $\vec{k}$. This would lead to overcounting of diagrams.[16] The restriction to diagrams with no positron-hole lines in the self-energy insertions forces one to omit diagrams like Fig. 2(b). The contribution of such diagrams vanishes, however, in the limit of low positron density. From Ref. 13 we note that it is correct to take the limit of low positron density before the other thermodynamic limits and (14) is therefore *exact*. Our discussion differs from that of Majumdar,[13] in that his prescription to omit diagrams with more than one hole line excludes diagrams such as Fig. 2(a), where the label of the hole line is repeated. Such diagrams give a nonvanishing contribution in the limit of low posi-

tron density.[17] We write

$$S(\vec{q},\vec{K},y_n)=\Sigma(\vec{q},y_n)+\lambda M(\vec{q},\vec{K},y_n)+O(\lambda^2) \quad , \quad (15)$$

where Σ is the position self-energy without any rooted vertex, so that (14) can be differentiated with respect to λ to give

$$E(\vec{K})=\frac{1}{N^+}\sum_{\vec{q}}\sum_{n=-\infty}^{\infty} G(\vec{q},z_n)M(\vec{q},\vec{K},y_n)e^{z_n 0+} \quad , \quad (16)$$

where

$$G(\vec{q},z_n)=T/[z_n-q^2-\Sigma(\vec{q},y_n)] \quad . \quad (17)$$

Pictorially, (16) corresponds to the sum of the "mug" diagrams of Fig. 3.

The Fourier coefficients $G(\vec{q},z_n)$ and $M(\vec{q},\vec{K},z_n-\mu)$ can be analytically continued as functions with a branch point at $z=\mu$. On the Riemannian sheet defined by a cut along the real axis there are no singularities off the axis,[18] and for large values of z the functions approach, respectively, z^{-1} and a constant. Since we have defined Σ and M not to include any hole lines, the branch cuts extend from $z=\mu$ only in the positive direction. When the positron-phonon interaction is taken into account this is, strictly speaking, not true, since the positron can emit and absorb thermal phonons, which will cause the cut to extend below $z=\mu$. There is no corresponding effect from the electron-positron interaction because we have used, following the argument below (8), $T=0$ distributions for the electrons. In our discussion we are primarily interested in positron momenta for which $q^2\sim T$, where $T\sim 100$–400 °K. In this region $q^2\gg qc$, where c is the sound velocity. Therefore, we may also neglect the discontinuities of Σ and M below $z=\mu$ for

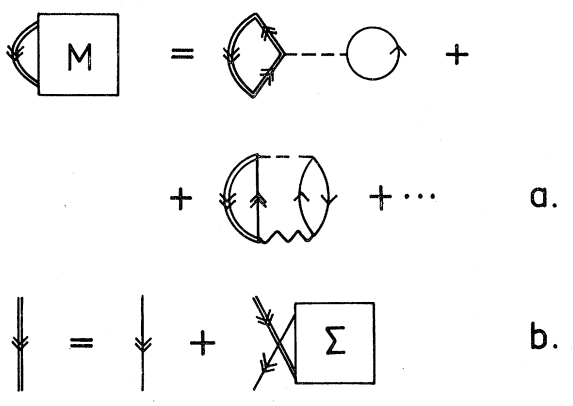

FIG. 3. Diagrams of the form given in Fig. 1 can be redrawn as "mug" diagrams. (a) The "handle" is made up of a positron-hole propagator, (b) which may contain any number of proper self-energy insertions, none of which contains any "rooted vertex." The "mug" proper is a proper self-energy insertion containing one "rooted vertex" (a).

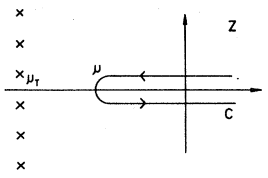

FIG. 4. Infinite sum in (16) can be transformed into an integral along the contour marked by C.

the positron-phonon interaction. In Sec. III we discuss assumptions 1–4 below.

Assumption 1. None of the quantities G, Σ, or M have any isolated poles on the real axis below the cut in the case of a homogeneous system.

We can now transform (16) into

$$E(\vec{K})=\frac{1}{2\pi i N^+}\sum_{\vec{q}}\int_C \frac{g^-(z-\mu_T)M(\vec{q},\vec{K},z-\mu)}{z-q^2-\Sigma(\vec{q},z-\mu)} \quad , \quad (18)$$

where the contour C is shown in Fig. 4 and

$$g^-(z-\mu_T)=1/[e^{(z-\mu_T)/T}+1]$$
$$=(8N^+\nu/3NT^{3/2}\pi^{1/2})\,e^{(z-\mu)/T}$$
$$+O((N^+/N)^2) \quad . \quad (19)$$

Here we have put

$$e^{\mu_0/T}=8N^+\nu/3NT^{3/2}\pi^{1/2} \quad , \quad (20)$$

where ν is a normalization constant to be determined by the requirement that there will be an equilibrium density of N^+/N positrons. In the noninteracting case (4), we have $\nu=1$. Writing

$$\Sigma(\vec{q},y+i\epsilon)=\Delta(\vec{q},y)\mp i\Gamma(\vec{q},y) \quad , \quad (21)$$

$$M(\vec{q},\vec{K},y\pm i\epsilon)=A(\vec{q},\vec{K},y)\mp iB(\vec{q},\vec{K},y) \quad , \quad (22)$$

we find

$$E(\vec{K})=(\nu/T^{3/2}\pi^{5/2})\int d^3q\int_0^\infty dy\; e^{-y/T}$$
$$\times\frac{\Gamma(\vec{q},y)A(\vec{q},\vec{K},y)+[y-q^2+\mu-\Delta(\vec{q},y)]B(\vec{q},\vec{K},y)}{[y-q^2+\mu-\Delta(\vec{q},y)]^2+\Gamma^2(\vec{q},y)} \quad , \quad (23)$$

where $\mu=\Delta(0,0)$.[15] We define

$$Z_{\vec{q}}=\left(1-\frac{\partial}{\partial y}\Delta(\vec{q},y)\Big|_{y=0}\right)^{-1} \quad , \quad (24)$$

$$m^*(\vec{q})=q^2Z_{\vec{q}}^{-1}[q^2+\Delta(\vec{q},0)-\mu]^{-1} \quad , \quad (25)$$

$$\tilde{\Gamma}(\vec{q},y)=Z_{\vec{q}}\Gamma(\vec{q},y) \quad . \quad (26)$$

When expanding in terms of a dynamically screened effective interaction one gets convergent integrals for $\Delta(\vec{q},y)$ and its derivative[3] with respect to y, at least in low-order perturbation theory, and there seems to be no reason for divergences in higher order. The signs of the leading terms are such as to prevent the denominators in (24) and (25) from blowing up.[19]

At moderately low temperatures the dominant contribution to the y integration in (23) comes from small values of y. It is then warranted to approximate $\Delta(\vec{q}, y)$ by the zero- and first-order terms in the Taylor expansion of this quantity with respect to y. Furthermore, we will argue in Sec. III:

Assumption 2. For moderately low temperatures we may approximate

$$A(\vec{q}, \vec{K}, y) \approx A(\vec{q}, \vec{K}, 0), \tag{27}$$

$$B(\vec{q}, \vec{K}, y) \approx 0. \tag{28}$$

This gives for (23)

$$E(\vec{K}) = [\nu/(\pi T)^{3/2}] \int d^3q Z_{\vec{q}}^* A(\vec{q}, \vec{K}, 0)\, \sigma(\vec{q}, T), \tag{29}$$

where we define the resolution (or smearing) function

$$\sigma(\vec{q}, T) = \frac{1}{\pi} \int_0^\infty \frac{\tilde{\Gamma}(\vec{q}, y)\, e^{-y/T}\, dy}{(y - q^2/m_{\vec{q}}^*)^2 + \tilde{\Gamma}(\vec{q}, y)^2}. \tag{30}$$

The positron-phonon contributions[5,6] to $Z_{\vec{q}}$ and $m_{\vec{q}}^*$ and also[20] $A(\vec{q}, \vec{K}, 0)$ have been estimated and found negligible. For a metal such as Na it is therefore justifiable to use estimates from electron-gas theory for all quantities in (29) and (30) *except* $\Gamma(\vec{q}, y)$.

Assumption 3. For moderate temperatures we may put

$$\sigma(\vec{q}, T) \approx e^{-q^2/m^* T}. \tag{31}$$

In Sec. III we argue that (31) holds well when only the electron-positron interaction is considered. As first pointed out by Mikeska, [6] the assumption breaks down when the positron-phonon interaction is included, causing a non-Boltzmann-like quasi-positron momentum distribution. In any case we can only have significant contributions to (30) for small momenta $\vec{q}$ at low temperatures. In the same sense as explained in the paragraph below (26), the quantities $Z_{\vec{q}}$ and $m_{\vec{q}}^*$ are well behaved and approach a constant value for small q, and we can, at low temperatures, use the $q = 0$ values for these quantities.

Assumption 4. For low temperatures we may approximate

$$A(\vec{q}, \vec{K}, 0) \approx A(0, \vec{K} - \vec{q}, 0). \tag{32}$$

We then get

$$E(\vec{K}) = [Z_0 \nu/(\pi T)^{3/2}] \int d^3q\, A(0, \vec{K} - \vec{q}, 0)\, e^{-q^2/m^* T}. \tag{33}$$

In Appendix A we show that

$$\nu = (m^*)^{-3/2}. \tag{34}$$

For $T = 0$, (30) becomes (as is shown independently in Appendix B)

$$\tilde{E}(\vec{K}) = Z_0 A(0, \vec{K}, 0). \tag{35}$$

Substituting (35) back into (33) finally gives (10). Since the phonon contribution to either side of (32) is negligible, [20] assumption 4 is quite innocent as far as this interaction is concerned. We must, however, take into account that (31) no longer is valid, and when the positron-phonon interaction is included, we obtain

$$E(\vec{K}) = (\pi m^* T)^{-3/2} \int d^3q\, \tilde{E}(\vec{K} - \vec{q})\, \sigma(q, T) \tag{36}$$

instead of (10). This equation is a natural generalization of Mikeska's result. [6]

III. VALIDITY OF ASSUMPTIONS

Assumption 1. In order to understand what is involved, consider the positron self-energy in the ladder (or t-matrix) approximation of Ref. 4:

$$\Sigma(\vec{q}, \omega) = \frac{16\beta}{3\pi N} \sum_{\vec{k}<1,\, \vec{p}>1} \frac{v(\vec{k}, \vec{p})\, t_{\vec{k}+\vec{q}, \vec{k}, \vec{p}}(\omega + k^2)}{\omega + k^2 - p^2 - (\vec{q} + \vec{k} - \vec{p})^2 + i\epsilon}, \tag{37}$$

where

$$t_{\vec{q}, \vec{k}, \vec{p}}(\omega) = \frac{8}{3\pi N} \left[v(\vec{p}, \vec{k}) - \sum_{\vec{s}>1} \frac{v(\vec{p}, \vec{s})\, t_{\vec{q}, \vec{k}, \vec{s}}(\omega)}{\omega - s^2 - (\vec{q} - \vec{s})^2 + i\epsilon} \right]. \tag{38}$$

A more complete theory would have the positron self-energy substituted self-consistently into all internal positron lines. This gives (neglecting the electron self-energy)

$$\Sigma(\vec{q}, \omega - \mu) = \frac{16\beta}{3\pi N} \sum_{\vec{k}<1,\, \vec{p}>1} \frac{v(\vec{k}, \vec{p})\, t_{\vec{k}+\vec{q}, \vec{k}, \vec{p}}(\omega + k^2)}{\omega + k^2 - p^2 - (\vec{q} + \vec{k} - \vec{p})^2 - \Sigma(\vec{q} + \vec{k} - \vec{p}, \omega - p^2 + k^2 - \mu)}, \tag{39}$$

$$t_{\vec{q}, \vec{k}, \vec{p}}(\omega) = \frac{8\beta}{3\pi N} \left[v(\vec{p}, \vec{k}) - \sum_{s>1} \frac{v(\vec{p}, \vec{s})\, t_{\vec{q}, \vec{p}, \vec{s}}(\omega)}{\omega - s^2 - (\vec{q} - \vec{s})^2 - \Sigma(\vec{q} - \vec{s}, \omega - s^2 - \mu)} \right]. \tag{40}$$

From a practical point of view, (39) and (40) may not be a very useful approximation since the numerical problem may be too tough to handle. The equations illustrate an important point, however, namely, that Dyson's equation

$$\epsilon(\vec{p}) = p^2 + \Delta(\vec{p}, \epsilon(\vec{p}) - \mu) \tag{41}$$

will not have any discrete solutions below the continuum. Suppose that such a solution exists for a given value of $\vec{p}$. Because of the homogeneous nature of the system such solutions must exist for a range of $\vec{p}$ values. When the corresponding self-energy is resubstituted into (40) and (41) the continuum is dragged down to the discrete level which

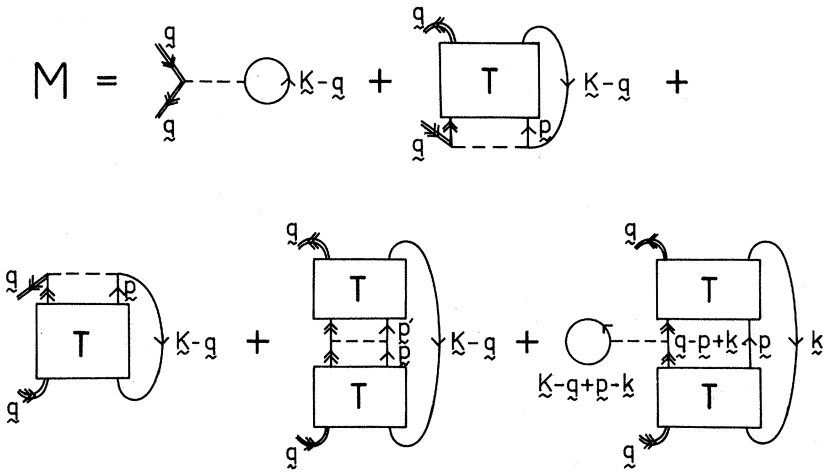

FIG. 5. Ladder approximation for the "mug," i.e., self-energy insertions with a rooted vertex. The box marked by T represents the t matrix.

thus no longer remains discrete. The argument also holds for $M(\vec{q}, \vec{K}, z-\mu)$, and in neither case is it limited to the particular diagrams we have considered.

We will later use the approximation (37) to illustrate our argument. We will not carry out the self-consistent program indicated by (39) and (40), but instead just shift the energies by the appropriate amount to avoid energy gaps. This was done in (37) and will be done without further comment in what follows.

We have discussed assumption 1 in some detail because one finds in the literature approximation procedures which lead to isolated poles in the t matrix. These have incorrectly been attributed to positroniumlike bound states. This need not mean that one cannot, in the low-electron-density limit, work with approximations[17,21] which explicitly introduce "bound states," as long as they are not taken too seriously.

Note that the argument that there are no isolated poles below the continuum need not hold for an inhomogeneous system, e.g., if the positron can be trapped at vacancy sites. In this case one would also expect a quite different temperature dependence of the angular correlation.

Assumption 2. In order to demonstrate the validity of (27) we must show that $A(\vec{q}, \vec{K}, y)$ is a slowly varying function of y over the range of y values for which the Boltzmann factor $e^{-y/T}$ is sizable. When considering temperatures $T \lesssim 400\,^{\circ}\mathrm{K}$ (roughly the melting temperature of sodium) this means that we are only interested in y values that are of the order 1% or less of the Fermi energy. In order to obtain order-of-magnitude estimates of the quantities involved, let us consider $M(\vec{q}, \vec{K}, y)$ in the approximation of Fig. 5. The last term is quite small. Using the effective interaction of Ref. 4, we have estimated the term to contribute, when integrated over $\vec{K}$, not more than 1% of the total enhancement. We consider it here in order to illustrate the behavior of contributions to the enhancement factor which, at $T=0$, are continuous at the Fermi surface. A high degree of cancellation must, however, be expected among such terms.[22] The first four terms in Fig. 5 can be summed up to give[23]

$$M_1(\vec{q}, \vec{K}, y) = \eta(1-|\vec{K}-\vec{q}|) \times\left[1-\sum_{\vec{p}>1}\frac{t_{\vec{K},\vec{p},\vec{K}-\vec{q}}(y+(\vec{K}-\vec{q})^2)}{y+(\vec{K}-\vec{q})^2-p^2-(\vec{K}-\vec{p})^2}\right]^2, \tag{42}$$

while the last term yields

$$M_2(q, K, y) = \sum_{k<1,\vec{p}>1}\frac{\eta(1-|\vec{K}-\vec{q}+\vec{p}-\vec{k}|)t^2_{\vec{k}+\vec{q},\vec{p},\vec{k}}(y+k^2)}{[y+k^2-p^2-(\vec{q}-\vec{p}+\vec{k})^2]}. \tag{43}$$

We first consider the y dependence of the real part of (42). Anticipating the discussion of assumption 4 we will only compare $A_1(0, \vec{K}, y)$ with $A_1(0, \vec{K}, 0)$. The y dependence of (42) cannot be expected to be sensitive to the details of the potential used in calculating the t matrix, as long as this only gives rise to reasonable electron-position correlations. We note that $\mathrm{Im}\,t_{\vec{K},\vec{p},\vec{K}}(y+K^2)$ vanishes unless $1>K>1-\frac{1}{2}y$. This range is insignificant for the small values of $y \sim T$ considered here. In the special case of the separable potential model of Ref. 4 we have

$$A_1(0, \vec{K}, y) = \eta(1-K)[1+\mathrm{Re}\,I(\vec{K}, y+K^2)]^{-2}, \tag{44}$$

where

$$I(\vec{q}, y) = \frac{\alpha\beta}{\pi^2}\int_{b>s>1}\frac{d^3s}{[y-s^2-(\vec{q}-\vec{s})^2+i\epsilon]} \tag{45}$$

and

$$\mathrm{Re}\, I(\vec{K}, y+K^2) = -\frac{a\beta}{\pi}\left(b - 1 - \frac{2b^2 - y - K^2}{2K}\ln\left|\frac{b^2 - Kb - \frac{1}{2}y}{b^2 + Kb - \frac{1}{2}y}\right|\right.$$
$$+ \frac{2 - y - K^2}{2K}\ln\left|\frac{1 - K - \frac{1}{2}y}{1 + K - \frac{1}{2}y}\right| + \frac{(K^2+2y)^{1/2}}{4}$$
$$\left.\times \ln\left|\frac{[b^2 - b(K^2+2y)^{1/2} + \frac{1}{2}y][1 + (K^2+2y)^{1/2} + \frac{1}{2}y]}{[b^2 + b(K^2+2y)^{1/2} + \frac{1}{2}y][1 - (K^2+2y)^{1/2} + \frac{1}{2}y]}\right|\right). \quad (46)$$

Since the derivative of (46) with respect to y is infinite for $K = 1$, we have checked numerically the y dependence of (44) and (45), using the parameter values $a = 0.0757$, $b = 8.22$, which at the sodium electron density ($\beta = 2.07$) gives the correct total displaced charge and the experimental sodium annihilation rate.[4] It was found that $A_1(0, \vec{K}, y)$ does not differ from $A_1(0, \vec{K}, 0)$ by more than 1%, when y amounts to 1% of the Fermi energy.

We have already mentioned that terms such as (43), which are continuous functions of $|\vec{K} - \vec{q}|$, are quite small. Their y dependence therefore represents a correction to a small correction, and cannot be expected to be important. We therefore conclude that the assumption (27) is valid. Just as is the case[5,6] with $\Delta(\vec{q}, y)$, the phonon contribution to $A(\vec{q}, \vec{K}, y)$ must be expected to be negligible, and, thus, inclusion of the electron-phonon interaction cannot affect our conclusions.

Turning to (28) we first consider terms such as (43) which are continuous functions of $|\vec{K} - \vec{q}|$. In the separable potential model of Ref. 4,

$$B_2(\vec{q}, \vec{K}, y) = \frac{\beta^2 a^2}{\pi^4}\,\mathrm{Im}\int \frac{\eta(1-k)\,d^3k}{1 + I(\vec{k}+\vec{q}, K^2 + y - i\epsilon)}$$
$$\times \int \frac{\eta(1 - |\vec{K} - \vec{q} + \vec{p} - \vec{k}|)\,d^3p}{[y + k^2 - p^2 - (\vec{q} - \vec{p} + \vec{k})^2]^2}$$
$$\approx \eta(1-K)\frac{\beta a}{\pi^2}\frac{\partial}{\partial y}\,\mathrm{Im}\int \frac{\eta(1-k)\,d^3k}{1 + I(\vec{k}+\vec{q}, y + k^2)}$$
$$\propto y \quad (47)$$

for small q. The result in (47) depends on the volume of phase space in which the energy denominator in (45) can vanish. The proportionality to y holds for any potential as long as a screened effective interaction, which is nonsingular for small momentum transfers, is used.

When only the interactions with the electrons are considered we find, in connection with the discussion of assumption 3, that $\Gamma(\vec{q}, y)$ is proportional to y^2 for small y. The dominant contribution to (23) then comes from y values $y \approx q^2/m^*(\vec{q})$ for which the factor in front of B in (23) vanishes. The effect of B_2 is then of the same order of magnitude as that of the higher derivatives with respect to y of $\Delta(\vec{q}, y)$ which we have ignored. When the positron-phonon interaction is taken into account one has instead $\Gamma(\vec{q}, y) \sim y^{1/2}T$. In this case, important contributions to (23) come from $y \lesssim T$, $q^2 \lesssim T$. The second term in the numerator of (23) will still be asymptotically small compared with the first.

The imaginary part of contributions, which are discontinuous at ($|\vec{K} - \vec{q}| = 1$) such as (42), also will be proportional to y for small y, but such terms vanish unless $1 - \frac{1}{2}y < |\vec{K} - \vec{q}| < 1$. Considering that the width associated with the resolution function (30) is of the order 10% of the Fermi momentum, when $T \sim 1\%$ of the Fermi energy the contribution from the imaginary part of (42) must be truly insignificant.

The phonon contribution to $B(\vec{q}, \vec{K}, y)$ is more conveniently treated in connection with the following discussion.

Assumption 3. The conclusion of our discussion of this assumption will be in qualitative agreement with previous results of Mikeska,[6] but our results are more general. The reader may find it helpful first to study the simpler cases discussed by Mikeska.[6] The same kind of argument as is used here has previously been applied by Luttinger,[18] and the limits of validity should be the same, i.e., our results are valid if many-body perturbation theory gives correctly analytical properties of self-energies near the quasiparticle energy. This has also been implicitly assumed elsewhere in the present paper.

We wish to study the properties of $\Gamma(\vec{q}, y)$ for small y. First consider the contribution from a given "skeleton graph," i.e., a graph not containing any self-energy insertions to internal lines. In this case no two internal lines have the same energy and momentum labels, so that zeros of energy denominators correspond to simple poles. The contribution to $\Gamma(\vec{q}, y)$ is then made up of δ-function contributions from the different energy denominators. These δ-function contributions will be proportional to the area of the hypersurface in phase space on which the denominators vanish. If the self-energies are substituted back self-consistently into the internal lines of the skeleton graph the arguments of the δ functions will, for small y, be the quasiparticle energies and not the bare energies.

When only electron interactions are taken into account the arguments of the δ functions contain contributions from the energies of the positron plus a number of electron-hole pairs. Clearly,[18] the

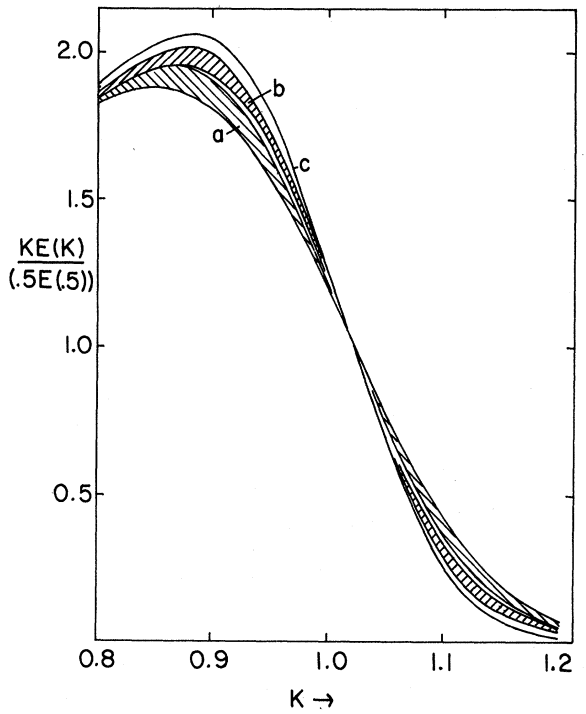

FIG. 6. Phonon effects on the thermal smearing. All curves are computed for $T=370\,^{\circ}\mathrm{K}$ and with (Ref. 2) $\tilde{E}(K)=1+0.34K^2+0.22K^4$. Curve c is obtained using (10) and $m^*=1.1$. The region a is delimited by curves obtained in the same way, but with $m^*=1.6$ and 2.0. The region b is delimited by curves obtained from (51), (30), and (36) with $\eta=1$ using, respectively, $Z_0=0.60$, $m^*=1.1$ and $Z_0=0.86$, $m^*=1.2$.

one-pair contribution dominates and from (8), for small positron momenta $\vec{q}$ and energy y, the area of the hypersurface is determined only by the electron-pair energy. This gives

$$\Gamma(\vec{q},\,y)\propto \int d^3k\,\eta(1-k)\int d^3p\,\eta(p-1)\delta(y-p^2+k^2) \propto y^2\,. \tag{48}$$

This result is not valid in a perturbation expansion in terms of the bare Coulomb interaction which is singular for small momentum transfer. When an expansion is made in terms of a more realistic dynamically screened interaction, this momentum region is dominated by a plasmon pole which cannot contribute to $\Gamma(\vec{q},\,y)$ for small y. It is easily seen, by taking the imaginary part of (37), that (48) also holds in an expansion in terms of a statically screened interaction in the t-matrix approximation.

We have estimated $\Gamma(q\approx 0,\,y)$ in the t-matrix approximation (37) using the separable potential model of Ref. 4 and the same values of the parameters as in the discussion of assumption 2. We found $\Gamma(q\approx 0,\,y)\approx 0.5\,y^2$. We substituted both this value and $2.0\,y^2$ into (30) and found that for $T\lesssim 400\,^{\circ}\mathrm{K}$ the deviation from (31) was insignificant compared to the effect of a 5% change in the effective mass in both cases.

As first pointed out by Mikeska[6] the picture changes when the positron-phonon interaction is taken into account. In the interesting temperature region we have

$$qc \ll q^2/m^* \sim T \ll E_F \tag{49}$$

for typical positron momenta q. Here c is the velocity of sound. The calculation of the phonon contribution to $\Gamma(\vec{q},\,y)$ involves the summation over δ-function contributions from energy denominators involving the positron plus a number of phonons. The first inequality means that for $y\sim T$ the phonon energy has little effect on the area of the hypersurface in phase space with vanishing energy denominators. This means that $\Gamma(\vec{q},\,y)$ will be proportional to

$$\int d^3q\,\delta(y-q^2)\sim\sqrt{y}\,. \tag{50}$$

The first inequality in (49) also indicates that it is justifiable to consider the phonons in the high-temperature limit. This gives rise to a factor of T from the phonon-distribution functions. Factors involving the ratio m/M of the electron and ion masses cancel in the leading term. To lowest order in the electron-phonon interaction one obtains[6,24]

$$\Gamma(\vec{q},\,y)=-\frac{Z_0\eta}{(2\pi)^3}\,\mathrm{Im}\int d^3p\int_{-\infty}^{+\infty}dx\int_{-\infty}^{+\infty}dz \times\frac{\mathrm{Im}\,D_R(\vec{q}-\vec{p},\,x)(-i\pi)\,\delta(z-p^2/m^*)[1+\coth(x/2T)]}{x+z-y-i\epsilon} \approx \tfrac{1}{2}\,Z_0\pi\eta T(m^*)^{3/2}y^{1/2}\,, \tag{51}$$

with

$$\mathrm{Im}D_R(\vec{k},\,x)=\tfrac{1}{2}\pi ck[\delta(x+ck)-\delta(x-ck)]\,. \tag{52}$$

Here η is a constant, proportional to the square of the positron-phonon interaction, and is unity when Thomas-Fermi theory is used for the screening of the ion-ion and positron-ion interactions. We use Debye theory and assume that the positrons only couple to longitudinal phonons. This is justifiable since, from (49), only phonons with low momenta are involved.

In Fig. 6 we have plotted the function $KE(\vec{K})$ using (51), (36), and (30) at $T=370\,^{\circ}\mathrm{K}$ and different values of Z_0 and m^*. The results are compared with curves obtained using (10) and different values of m^*. We see that for reasonable values of the parameters, $\Gamma(\vec{q},\,y)$ will be too large for (31) to be valid.

Corrections to (51) arising from multiphonon contributions will involve higher powers of T arising from the phonon distribution function $[1+\coth(x/2T)]$. As a check that such contributions are negligible we have evaluated (51) substituting $\Gamma(\vec{q},\,y)$ self-

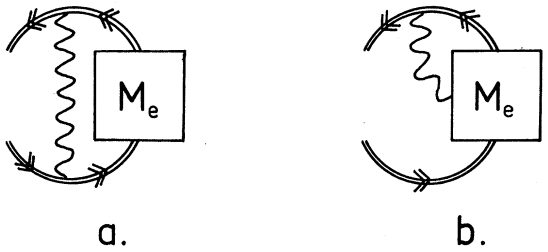

FIG. 7. Contributions to M from the positron-phonon interaction. Here M_e is the contribution from electron-positron interaction only. The wavy line represents a phonon.

consistently into the positron propagator. In the limit (49) this gives

$$\Gamma(\vec{q}, y)=\frac{\eta T}{4}\int_{p<k_D} d^3p \frac{\Gamma(\vec{p}-\vec{q}, y)}{(y-|\vec{p}-\vec{q}|^2/m^*)^2+\Gamma^2(\vec{p}-\vec{q}, y)}, \tag{53}$$

where k_D is the Debye momentum. For small values of T, y, and q, (53) has the solution

$$\Gamma(\vec{q}, y)=\gamma(y+\tfrac{1}{4}\gamma^2), \tag{54}$$

$$\gamma=\tfrac{1}{2}\eta\pi(m^*)^{3/2}T. \tag{55}$$

We have found that the change in the thermal smearing, when (54), (55) was substituted instead of (51) into (36) and (30), would not be visible in Fig. 6. The electron-positron interaction affects the parameters Z_0, η, and m^*. From (48) we can, however, neglect the contribution to $\Gamma(\vec{q}, y)$ from energy denominators involving electron-hole pairs.

We next turn to the phonon contribution to $B(\vec{q}, \vec{K}, y)$, the imaginary part of $M(\vec{q}, \vec{K}, y)$. Because of the order-of-magnitude difference between (48) and (51) we need only to consider δ-function contributions from energy denominators involving positrons and phonons. Consider[24] first the diagram in Fig. 7(a). It gives

$$M_{7(a)}(\vec{q}, \vec{K}, y)$$

$$=\frac{-\eta}{(2\pi)^3}\int d^3p\int_{-\infty}^{+\infty}dx\int_{-\infty}^{+\infty}dz\,\frac{\mathrm{Im}D_R(\vec{q}-\vec{p}, x)}{x+z-y-i\epsilon}$$

$$\times\mathrm{Im}\left[\frac{M_e(\vec{p}, \vec{K}, z)}{(z-p^2/m^*+i\epsilon)^2}\right][1+\coth(x/2T)]. \tag{56}$$

Here M_e is the contribution to M from the electron-positron interaction alone and from (49), (51), (52), and (56)

$$B_{7(a)}(\vec{q}, \vec{K}, y)\approx-\frac{\partial}{\partial y}A(\vec{q}, \vec{K}, y)|_{y=0}\Gamma(\vec{q}, y), \tag{57}$$

where A is the real part of M_e.

From the discussion of Appendix A we note that affixing a phonon line to a positron line is, in the limit of low phonon energy and momentum, equivalent to differentiation of $M(\vec{q}, \vec{K}, y)$ with respect to y. We therefore expect the diagram in Fig. 7(b) to give a contribution similar to (57). From (23) we see that the effect of neglecting the term (57) is essentially the same as neglecting the y dependence of $A(\vec{q}, \vec{K}, y)$ for small values of y. This was justified in connection with the discussion of assumption 2. We therefore conclude that the approximation involved in (28) is reasonable and phonons will thus affect the positron thermal motion only through Eq. (51).

Assumption 4. The approximation involved in (32) is worst for terms which are discontinuous at $|\vec{K}-\vec{q}|=1$. Since the discontinuities of $A(\vec{q}, \vec{K}, y)$ and $A(0, \vec{K}-\vec{q}, y)$ coincide, the validity of the assumption depends on the effect of the difference between the energy denominators in these two cases. This difference involves terms proportional to q^2 and $\vec{q}\cdot\vec{K}$. The former can be ignored by arguments similar to the discussion of assumption 2. Unfortunately, the $\vec{q}\cdot\vec{K}$ terms do not average to zero in the angular integrations because of Fermi-surface restrictions. We therefore felt that a numerical check of (32) was needed. As before, we used the separable potential model of Ref. 4 and the same values of the parameters. Without making use of (32) we would have

$$E(\vec{K})=\frac{Z_0\nu}{(\pi T)^{3/2}}\int d^3p\,\frac{\eta(1-p)\sigma((\vec{p}-\vec{K}), T)}{[1+I(\vec{K}, p^2)]^2}, \tag{58}$$

where $I(\vec{K}, p^2)$ can be obtained from (46). If (32) is valid, then (56) should be approximately equal to

$$\frac{Z_0\nu}{(\pi T)^{3/2}}\int d^3p\,\frac{\sigma(\vec{p}-\vec{K}, T)\eta(1-p)}{[1+I(\vec{p}, p^2)]^2}. \tag{59}$$

We found that (58) gives rise to a slightly smaller enhancement factor near the Fermi momentum than (59) does. At $T=600$ °K and $\sigma(\vec{q}, T)=e^{-q^2/1.8T}$ the effect would be indistinguishable from that of a 0.5% reduction in the Fermi momentum. The effect is even smaller at low temperatures, and considerably smaller than that of the thermal expansion which actually takes place. Since the numerical method of Stewart and co-workers compensates for thermal expansion, we feel that the approximation involved in assumption 4 does not affect the interpretation of the experiments.

IV. DISCUSSION

We have shown that when the electron-positron, electron-electron, and positron-phonon interactions are taken into account, the thermal smearing of the angular correlation is, at moderate temperatures, given by (51), (36), and (30). The computation of the angular correlation at a given temperature then requires the knowledge of the zero-temperature angular correlation $\tilde{E}(\vec{K})$, the quasipositron renor-

malization constant Z_0, the positron effective mass m^*, and the electron-phonon coupling strength η.

In Fig. 6 we compare theoretical curves obtained for $T = 370\,^\circ\mathrm{K}$ using a phenomenological[2] zero-temperature angular correlation $\tilde{E}(\vec{K})$. The region marked a represents the thermal smearing which is compatible with an "apparent" effective mass of 1.8 ± 0.2, which is the quoted experimental value for Na. From previous calculations[3,4] one would expect the effective mass, including the band contribution,[2,7] to lie in the range $m^* = 1.1$–1.2 for Na. Mikeska[6] quotes a value $Z_0 = 0.60$ while the calculation in Ref. 4 gives $Z_0 = 0.86$. From the discussion of Ref. 6, the relative uncertainty in η is probably of the same order as the uncertainty in Z_0. In the case $\eta = 1$, $m^* = 1.1$, and $Z_0 = 0.6$, the phonon effects enhance the apparent effective mass by 15%, while for $\eta = 1$, $m^* = 1.2$, $Z_0 = 0.86$, the enhancement is roughly 30%. With the latter choice of parameters the discrepancy between theory and experiment is sufficiently small that one hesitates to make categorical statements about their incompatibility. For this reason we feel it would be highly desirable if the experimental uncertainty could be reduced by new experiments. On the theoretical side it should be possible to determine the parameter η and the factor $Z_0(m^*)^{3/2}$ more accurately and calculations should be made for all the alkali metals.

ACKNOWLEDGMENTS

We are very grateful to S. M. Kim for many helpful discussions on the correct interpretation of the experiments involved, and to J. P. Carbotte and to T. McMullen for stimulating discussions.

APPENDIX A: DETERMINATION OF ν

We can determine the mean positron number N^+ in the ensemble by adding a term

$$\lambda_1 \sum_{\vec{p}} b_{\vec{p}}^\dagger b_{\vec{p}} \tag{A1}$$

to the Hamiltonian and evaluating

$$N^+ = \frac{\partial \Omega}{\partial \lambda_1}\bigg|_{\lambda_1=0} = \frac{1}{2\pi i}\sum_{\vec{q}} \int_c \frac{g^-(z-\mu_T) M_1(\vec{q}, z-\mu)}{z - q^2 - \Sigma(\vec{q}, z-\mu)}\, dz\,. \tag{A2}$$

Here M_1 is the sum of all self-energy insertions containing a "rooted vertex" (A1). One contribution to M_1 contains nothing but the rooted vertex, in which case we have

$$M_1^q(\vec{q}, z-\mu) = 1\,. \tag{A3}$$

The remaining contributions to M_1 all have a rooted vertex attached to a positron line in a proper self-energy insertion. The propagator to which the rooted vertex is attached is then modified according to

$$\frac{1}{z-q^2} \to \frac{1}{(z-q^2)^2} = -\frac{\partial}{\partial z}\frac{1}{z-q^2}\,. \tag{A4}$$

Summing up all the ways the rooted vertex can be attached gives

$$M_1(\vec{q}, z-\mu) = 1 - \frac{\partial}{\partial z}\Sigma(\vec{q}, z-\mu)\,. \tag{A5}$$

Substituting (A5) into (A2) and grinding the expression through the same machinery as in Sec. II gives (34). Note that because of the difference between S and $\tilde{S}$ [see the paragraph below (14)], the usual expression for particle number

$$\frac{1}{2\pi i}\sum_{\vec{q}} \int_c \frac{g^-(z-\mu_T)\, dz}{z - q^2 - \Sigma(\vec{q}, z-\mu)} \tag{A6}$$

will not give the correct answer.

APPENDIX B: ZERO-TEMPERATURE THEORY

In this case it is convenient to work with a 1-positron N-electron system. The unperturbed system then contains one zero-momentum positron in the Fermi sea. Analogous to the previous discussion we add a term $\lambda P(\vec{K})$ to the Hamiltonian and evaluate

$$\tilde{E}(\vec{K}) = \frac{\partial E}{\partial \lambda}\bigg|_{\lambda=0}\,, \tag{B1}$$

where E is the ground-state energy. We have

$$\tilde{E}(\vec{K}) = \frac{\partial}{\partial \lambda}\bigg|_{\lambda=0} \times \frac{1}{2\pi i}\sum_{l=1}^{\infty}\frac{1}{l}\int_{-\infty}^{\infty} dy\, e^{iy0^+}\frac{[S(0, \vec{K}, y-\mu)]^l}{(y - i\epsilon)^l}\,. \tag{B2}$$

Here $S(0, \vec{K}, y-\mu)$ is the sum of all proper self-energy insertions (with or without a rooted vertex) to a zero-momentum positron-hole line. Up to terms which can be neglected in the limit of infinite volume, no proper self-energy insertion contains any positron-hole line. $S(0, \vec{K}, y-\mu)$ is therefore analytic in the upper half of the complex y plane. From (15), summing up and reexpanding a geometrical series, using $\mu = \Sigma(0, 0)$ and the analyticity in the upper half of the y plane, we get

$$\begin{aligned}\tilde{E}(\vec{K}) &= \frac{1}{2\pi i}\sum_{l=1}^{\infty}\int_{-\infty}^{\infty} dz\, e^{iz0^+} M(0, \vec{K}, z)\frac{[\Sigma(0, z) - \mu]^{l-1}}{(z - i\epsilon)^l} \\ &= \sum_{l=1}^{\infty}\frac{1}{(l-1)!}\frac{d^{l-1}}{dz^{l-1}} \\ &\quad \times \{M(0, \vec{K}, z)[\Sigma(0, z) - \Sigma(0, 0)]^l\}\big|_{z=0} \\ &= Z_0 M(0, \vec{K}, 0)\,.\end{aligned} \tag{B3}$$

Since $M(0, \vec{K}, 0)$ is real, (B3) and (35) agree.

*Research supported in part by the National Research Council of Canada, the Emil Aaltonen Foundation, and Academia Scientarium Fennica.

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[15]We have, as in Ref. 4, *defined* the self-energy as a function of the energy relative to μ. This notation helps us remember that, if one cannot substitute the self-energy self-consistently in the appropriate skeleton diagram, one must shift the energies of internal lines by the amount μ. Otherwise one gets nonphysical energy gaps, as in the calculation of Arponen (Ref. 21).

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[23]In the usual ladder approximation [S. Kahana, Phys. Rev. 129, 1622 (1963)], one omits what in our formalism appears as self-energy corrections to the "handle" in Fig. 3. At low temperatures this corresponds to a factor Z_0, but it has been pointed out (Ref. 17) that the error one makes in neglecting this factor largely cancels with vertex corrections to this ladder approximation. In Ref. 4 the factor Z_0 was neglected, for this reason, in estimates of the annihilation rate.

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