POSITRON ANNIHILATION IN METALS

A THESIS
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TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Chapter</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>The Hamiltonian and the Green's Functions</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>Formal Theory of Annihilation</td>
<td>22</td>
</tr>
<tr>
<td>3</td>
<td>Kahana's Theory of Positron Annihilation</td>
<td>37</td>
</tr>
<tr>
<td>4</td>
<td>Effect of Particle-Hole Interactions on the Annihilation Rates</td>
<td>53</td>
</tr>
<tr>
<td>5</td>
<td>Effect of Self Energies on the Angular Correlation Curve for Momenta Smaller Than the Fermi Momentum</td>
<td>75</td>
</tr>
<tr>
<td>6</td>
<td>Effectiveness of Electron-Electron Interactions at Producing Tails in the Angular Distribution Curve</td>
<td>85</td>
</tr>
<tr>
<td>7</td>
<td>Effect of the Lattice on Positron Annihilation in Sodium</td>
<td>116</td>
</tr>
<tr>
<td>8</td>
<td>Thermalization Time of a Positron in a Metal</td>
<td>132</td>
</tr>
<tr>
<td>Appendix 1</td>
<td></td>
<td>145</td>
</tr>
<tr>
<td>Appendix 2</td>
<td></td>
<td>148</td>
</tr>
<tr>
<td>Appendix 3</td>
<td></td>
<td>154</td>
</tr>
<tr>
<td>Appendix 4</td>
<td></td>
<td>161</td>
</tr>
<tr>
<td>Appendix 5</td>
<td></td>
<td>167</td>
</tr>
<tr>
<td>Appendix 6</td>
<td></td>
<td>171</td>
</tr>
<tr>
<td>Appendix 6: A Short Note on Beryllium</td>
<td>130</td>
<td></td>
</tr>
<tr>
<td>References:</td>
<td>180</td>
<td></td>
</tr>
</tbody>
</table>
INTRODUCTION

The theory of positron annihilation in condensed matter was reviewed in 1956 by R.A. Ferrell and again in 1960 by P.R. Wallace. There is therefore little need to give a detailed historical survey of its development; we will limit ourselves to a brief summary of the state of the theory as reviewed by Ferrell and then pass immediately to a discussion of some of the more recent work which has a direct bearing on this thesis.

In a typical positron annihilation experiment, a high energy positron from some $\beta^+$ decay source penetrates deep into a thin metal sample and quickly becomes thermalized. This low energy positron then "migrates" through the sample and eventually annihilates with one of the metallic electrons with subsequent emission of two quanta. The annihilation radiation is of high energy (approximately 1 M.e.v.) and so can leave the metal sample relatively unattenuated and unscattered. It is this radiation which is finally detected and analysed. Two measurements can be made:

1. the total annihilation rate, and
2. the angular correlation of the two gamma-rays.

The first angular correlation measurements for a metal were carried out by S. de Benedetti and H.J. Richings, while total rates were determined by R.E. Bell and R.L. Graham. Later, much new experimental data became available (see Wallace's review). Experimentally, the angular correlation curve for many metals is an inverted parabola with small "tails" extending beyond the natural cut-off for this parabolic distribution. Except for the "tails", this is precisely the type of distribution expected on a
simple Sommerfeld model (see Chapter 2) for annihilation with the valence electrons only. De Benedetti, and later Ferrell, argued that a thermalized positron should be effectively excluded from the core and that we would indeed expect annihilation with only the valence electrons. Further if the positron Bloch type wave function is to be zero inside the core, there must necessarily be high momentum components present in this wave function. This could explain the tails.

The Sommerfeld model predicts total rates proportional to the valence electron density. This does not agree with the experimental results. Not only does the Sommerfeld theory predict rates which are much too small for most metals, but it also gives too large a variation from metal to metal. To remove this discrepancy, Ferrell suggested that the screened coulomb force between the annihilating electron-positron pair be taken into account. He took this screened force from a Bohm-Pine analysis and argued that this weakened interaction should admit of a perturbation treatment, which he carried to first order. (He also incorporated the Pauli Principle in his calculation.) This led to rates which are increased over their Sommerfeld value and which do not vary as much with electron density. Further, the enhancement factor is reasonably constant across the Fermi sea, thus leaving the angular correlation curve unaffected. This seemed to be a step in the right direction.

The next significant development was made by S. Kahana. He wrote down and solved a Bethe-Goldstone type equation for an electron-positron pair immersed in an electron gas, which incorporated both the Pauli Principle and the screened coulomb force. In this way he obtained total rates in reasonable agreement with available experimental data, and he also found that the angular correlation curve is unaffected. However, when the more precise
experimental values of R.E. Bell and M.H. Jorgensen\(^{(9)}\) became available, it was recognized that the theoretical rates of K-I were too large by a factor of 2. This prompted Kahana to redo the calculation of K-I, using a better model for the screened force.\(^{(9)}\) This yielded rates in very good agreement with experiment. (See figure 2-2.)

Up to now we have been concerned solely with the problem of accounting for the electron-positron force. There are however two important papers concerned mostly with the angular correlation problem which must be mentioned. They are the independent work of E. Daniel\(^{(9)}\), and of S. Berko and J.S. Plaskett\(^{(10)}\). In both these papers the positron wave function in copper was determined by using a Wigner-Seitz method. (Aluminium was also considered by Berko and Plaskett.) Expanding this wave function in a Fourier series they found that the higher momentum components have very small coefficients and that they certainly cannot account for the experimental tails. In other words, the positron wave function is not excluded from the core as much as was expected by Ferrell. Further, using the positron wave function they calculated core annihilation on a rigid ion model and found that it introduces long and broad tails. They concluded that core annihilation is responsible for the major part of the experimental tails.

The result of Berko and Plaskett, that core annihilation is responsible for the tails, coupled with Kahana's results for the valence electrons, give an adequate explanation of the main features of positron annihilation in many metals, and any further theoretical refinement can be expected to deal with quantities which are rather small as compared with the large enhancement
factors given in K-II. These refinements can be of two types. First we can try to better understand the effect of the positron force on a fully interacting valence electron gas. Secondly, we can try to improve the model of the metal, i.e. include the lattice. This thesis will be concerned mostly with the first of these, although the lattice is included in some of the formalism, and Chapter 7 deals entirely with the effect of the lattice in sodium.

Since we intend to approach the problem using modern Green's function techniques (as Kahana did), we begin by generalizing the well known formalism for a many-Fermion system to include both the positron force and the lattice potential. The partial annihilation rate \( Q_\omega \) (i.e. the probability of annihilation with emission of a photon pair of total momentum \( \omega \)) is then related to one of these Green's functions, specifically the electron-positron correlation function. This gives \( Q_\omega \) in the most general case as a set of Feynman graphs, with a prescription to translate each graph into a concrete mathematical expression.

Next, it is shown that many of these graphs contribute nothing to \( Q_\omega \) and so can be dropped. There still remain a large number, and Kahana's method immediately appears to be one of selective summation of diagrams. That is, of the totality of Feynman graphs representing \( Q_\omega \), only a small subset are summed, namely the ladder graphs (to all orders). Thus the question arises, why is Kahana's theory so successful? We must mention here the work of a Japanese group who essentially generalized the work of K-I to include positron - electron hole interactions as well as positron-electron interactions, and thus arrived at rates significantly less than those given in K-I. Further, it is known from the
combined work of K-I and K-II that the annihilation rates are quite sensitive to the choice of the effective potential. Hence it is important to understand why the static limit of the effective potential \( \omega(q, \omega) \) as used in K-II gives such good results. This is especially critical in the region around the Fermi surface where there is a large concentration of electrons. Very closely connected with this problem is the question of the real momentum distribution in a fully interacting electron gas, i.e. electron self energies. One would think that these would smooth out the variation of the enhancement factor across the sea by reducing it more in the region around the Fermi surface than at the center. (So should positron self energies.) Moreover there is the possibility that electron self energies can produce tails in the angular distribution. Stewart's experimental paper on the Fermi surface for sodium\(^{11} \) has influenced our thinking on this point. If the electron gas "inverted parabola" as given in K-II is super-imposed on the core annihilation curve from Chapter 7, one expects a sharp break at \( \epsilon = \epsilon_c(q = q_F, \text{the Fermi momentum}) \). (This is still expected when the lattice is included. See Chapter 7.) In the experimental curve this discontinuity would of course be smoothed out somewhat by the instrument resolution. However, Stewart claims that when a correction is made for this, the discontinuity is still not as sharp as would be expected. He deduces from this that either there is a "bump" in the Fermi surface, or else this is evidence of the effect of electron-electron interactions.

All these questions are considered in the course of this thesis. In attempting to answer them we are led to make an estimate of the effect on \( Q_q \) of all Feynman diagrams consistently up to second order, in addition to some higher order graphs which
form a natural group with one or more of the second order ones.

Summary of the more important results.

In Chapter 3, Kahana's theory is reviewed. The effective electron-positron potential is derived with the lattice included, although no use is made of it in calculations. An expression for the total annihilation rate in the high density limit, including both continuum and plasmon contributions, is given and evaluated numerically. The Bethe-Goldstone type equation needed to extend the theory to lower densities is derived and re-evaluated numerically, to check on the variation of the total rates with electron density in the region \( n \approx 2 \), where Kahana's curve increases a little faster than the experimental curve. We agree with the variation given in K-II.

The problem of the variation of \( \mathcal{R}_p \) across the sea in the high density limit is also considered in this chapter. It is found that replacing the full dynamic potential \( \mathcal{V}(\chi; \omega) \) in the first order ladder graph by its static limit tends to underestimate the variation of \( \mathcal{R}_p \) across the sea. However, in Chapter 5 it is found that this error is compensated for by the self energy effects. In other words, Kahana's enhancement factors can be thought of as already including self energy effects. Thus the static potential is even more appropriate for the problem at hand than originally expected.

In Chapter 4 we are concerned with hole-particle interactions. It is found that these are negligible, not so much because positron - electron hole interactions amount to only a small reduction of \( \mathcal{R} \) (the total rate), but rather because there also exists the possibility of electron - electron hole interactions, which
carry the opposite sign; these two contributions cancel to a large extent.

In Chapter 6 the possibility of tails coming from electron self energies is examined. First all enhancement effects are neglected and then the theory is extended to include these. Our final result is that no tails would show up experimentally because the incoming positron is effectively kept from sampling an electron with momentum $q > q_*$ by the screening charge which must necessarily exist in its surroundings.

In Chapter 7 the effect of the lattice in sodium is examined. It is found that core annihilation is mostly responsible for the tails, with conceivably a small percentage coming from the high momentum components in the electron Bloch states (and even less coming from the excluded volume effect). The question of an enhancement factor for core annihilation is raised, but no calculation is given. An enhancement factor of about 3 seems reasonable and would give good agreement with experiment.

In Chapter 8 an alternate expression to that of Lee-Whiting for the thermalization time is derived, using Green’s functions. In a certain limit our expression is shown to reduce to Lee-Whiting’s result; however, in its general form it has the advantage that it does not involve an arbitrary cut-off in the effective electron-positron potential function.
Chapter 1

THE HAMILTONIAN AND THE GREEN'S FUNCTIONS

THE HAMILTONIAN

We will work entirely within the framework of second quantization. The system we wish to describe consists of an electron gas probed by a positron, the whole immersed in a metallic lattice. As Hamiltonian for this system of electrons and positrons we take

\[
H = \int d^3x \, \psi^*(\mathbf{x}) (-\nabla^2 + V_e(\mathbf{x})) \psi(\mathbf{x}) + \int d^3x \, \phi^*(\mathbf{x}) (-\nabla^2 + V_p(\mathbf{x})) \phi(\mathbf{x}) \\
+ \frac{1}{2} \int d^3x \, d^3x' \, \psi^*(\mathbf{x}) \psi^*(\mathbf{x}') \mathcal{V}(\mathbf{x}, \mathbf{x}') \psi(\mathbf{x}) \psi(\mathbf{x}') \\
+ \frac{1}{2} \int d^3x \, d^3x' \, \phi^*(\mathbf{x}) \phi^*(\mathbf{x}') \mathcal{V}(\mathbf{x}, \mathbf{x}') \phi(\mathbf{x}) \phi(\mathbf{x}') \\
- \int d^3x \, d^3x' \, \psi^*(\mathbf{x}) \phi^*(\mathbf{x}') \mathcal{V}(\mathbf{x}, \mathbf{x}') \psi(\mathbf{x}) \phi(\mathbf{x}')
\]

(1)

where \( \psi(\mathbf{x}) \) is the electron field operator in the Schrödinger picture and \( \psi^*(\mathbf{x}) \) is its Hermitian conjugate. Similarly, \( \phi(\mathbf{x}) \) is the positron annihilation operator with adjoint \( \phi^*(\mathbf{x}) \). The two body interaction function \( \mathcal{V}(\mathbf{x}, \mathbf{x}') \) is the familiar Coulomb potential. Further, \( V_e(\mathbf{x}) \) is some average crystal field seen by an electron which enters the theory as an external potential. Nothing more about \( V_e(\mathbf{x}) \) need be specified at this stage, except that it must have the periodicity of the metallic lattice, i.e., \( V_e(\mathbf{x} + \mathbf{J}_i) = V_e(\mathbf{x}) \) where \( \mathbf{J}_i \) is a primitive translation vector for the lattice of the particular solid under consideration. Of course the exact nature of \( V_e(\mathbf{x}) \) is ultimately of great interest since it is through \( V_e(\mathbf{x}) \) that the solid state surroundings of the electron-positron gas
enter into the mathematical formalism. We will return to a more
detailed description of \( V_e(x) \) when we discuss a specific example
(sodium). The function \( V_p(x) \) is a similar potential for the posi-
tron. Finally, we will use units in which Planck's constant \( \hbar \) is
equal to 2\( \pi \) and the electron mass is \( \frac{1}{2} \), i.e. \( \hbar = 2\pi = 1 \).

The statistics appropriate to Fermions are expressed by the
anticommutation rules:

\[ \{ \psi(x), \psi^*(x') \} = \delta(x-x') \quad \{ \psi(x), \psi(x') \} = 0 \]  
\[ \{ \phi(x), \phi^*(x') \} = \delta(x-x') \quad \{ \phi(x), \phi(x') \} = 0 \]

\[ \text{c). every electron operator anticommutes with every positron } \]
operator.

As written, the Hamiltonian (1-1) is invariant under the sim-
ultaneous interchange of

a) electron and positron field operators

b) the periodic potentials \( V_e(x) \) and \( V_p(x) \).

Our system which consists of a single positron and a whole sea of
electrons is of course not symmetric in electrons and positrons.
But this asymmetry enters the theory only through the state vec-
tors and not through the operators. Advantage can be taken of
this situation to develop a formalism in most of which electrons
and positrons enter in a symmetric way.

Neglecting the periodic potential \( V(x) \) means essentially
smearing out the charge, concentrated about the various lattice
sites (at \( R_m = m \frac{a}{2} \)), into a uniform fixed background
of positive charge which serves to neutralize the negative charge
of the electron gas. In this approximation two metals differ
only through their valence-electron density. This is certainly
an idealization. It is however a very useful one since it intro-
duces complete translational invariance in a system which other-

wise possesses only the weaker symmetry of invariance under finite translation through a primitive lattice vector \( \mathbf{\ell}_i \). More precisely, when \( V(\mathbf{q}) \) is neglected the linear momentum operator \( \mathbf{Q} \) which is the generator for infinitesimal translations commutes with the Hamiltonian and hence also the unitary operator \( \mathbf{i} \mathbf{Q} \) for arbitrary \( \mathbf{q} \). On the other hand, when \( V(\mathbf{q}) \) is accounted for only \( \mathbf{i} \mathbf{Q} \) commutes with \( \mathbf{H} \). Denote this operator by \( \mathcal{T}_i \). Then

\[
\mathcal{T}_i = \mathcal{i} \mathbf{Q} \mathbf{Y}_i
\]  

and we assert that, from general symmetry principles,

\[
[\mathbf{H}, \mathcal{T}_i] = 0
\]

It is often useful to introduce a description of the system in terms of Bloch states. This is accomplished by introducing the decomposition of the Heisenberg field operators,

\[
\psi(\mathbf{r}) = \sum_{\mathbf{k} \in \mathbb{R}^3} \psi_{\mathbf{k} \mathbf{q}}(\mathbf{r}) \mathbf{Q}_{\mathbf{k} \mathbf{q}}(\mathbf{r})
\]

\[
\phi(\mathbf{r}) = \sum_{\mathbf{k} \in \mathbb{R}^3} \phi_{\mathbf{k} \mathbf{q}}(\mathbf{r}) \mathbf{Q}_{\mathbf{k} \mathbf{q}}(\mathbf{r})
\]

where the \( \psi_{\mathbf{k} \mathbf{q}}(\mathbf{r}) \)'s are the Bloch states appropriate to the electrons. They are simultaneous eigenstates of the Hamiltonian operator \( \mathbf{H} + \mathbf{V} \) belonging to the eigenvalues \( E_{\mathbf{k} \mathbf{q}} \) and of the translation operator \( \mathbf{Q}_{\mathbf{k} \mathbf{q}}(\mathbf{r}) \) belonging to the eigenvalues \( \mathbf{i} \mathbf{k} \cdot \mathbf{Y}_i \). Hence they can be written in the form

\[
\psi_{\mathbf{k} \mathbf{q}}(\mathbf{r}) = \frac{1}{V} \mathbf{i} \mathbf{k} \cdot \mathbf{r} \psi_{\mathbf{k} \mathbf{q}}(\mathbf{r})
\]

where \( V \) is the crystal volume and \( \psi_{\mathbf{k} \mathbf{q}}(\mathbf{r}) \) possesses the periodicity of the lattice. (Similarly the \( \phi_{\mathbf{k} \mathbf{q}}(\mathbf{r}) \)'s equal to \( \frac{1}{V} \mathbf{i} \mathbf{k} \cdot \mathbf{r} \phi_{\mathbf{k} \mathbf{q}}(\mathbf{r}) \) are the Bloch states for the positron.) The indices \( (\mathbf{k}) \) are the quantum numbers needed to label the various eigenstates of \( -\mathbf{V}^2 + \mathbf{V} \) in the reduced zone scheme. In this scheme the reciprocal lattice space, or "\( \mathbf{k} \)-space", is divided up into various regions called
Brillouin zones. These are numbered by the zone index \( l \) which ranges over the natural numbers. The index \( \mathbf{k} \), on the other hand, ranges over the first Brillouin zone. For a finite crystal with \( N_i \) cells in the \( \mathbf{i}_i \) direction, \( \mathbf{k} \) is further restricted to a discrete set within the first zone by imposing periodic boundary conditions on the crystal faces, i.e.

\[
\mathbf{k} = n \mathbf{i}_i \quad \text{for arbitrary integral } n_i
\]

with restriction to the first zone understood.

The Bloch states \( \Psi_{\mathbf{k}, n}(x) \) are an orthonormal set of functions in the inner product

\[
\langle \mathbf{k}, \mathbf{l}, n; \mathbf{k}', \mathbf{l}', n' | \mathbf{k}, \mathbf{l}, n; \mathbf{k}', \mathbf{l}', n' \rangle = \delta_{\mathbf{k}, \mathbf{k}'} \delta_{n, n'} \delta_{l, l'}.
\]

They are a complete set in the space of periodic functions with periodicity \( N_i \mathbf{i}_i \) in the \( \mathbf{i}_i \) direction. Finally, in the limit when the crystal volume tends to infinity, all sums over \( \mathbf{k} \) go over into integrals according to the rule

\[
\frac{1}{V_\mathbf{k}} \longrightarrow \frac{1}{(2\pi)^3} \int d^3 \mathbf{k}
\]

* The \( \mathbf{i}_i \)'s are the primitive translation vectors for the reciprocal lattice, defined by \( \mathbf{a}_1 = \mathbf{i}_x \mathbf{i}_y / L_x \), \( \mathbf{a}_2 = \mathbf{i}_y \mathbf{i}_z / L_y \), \( \mathbf{a}_3 = \mathbf{i}_z \mathbf{i}_x / L_z \) where \( L = V \mathbf{i}_1 \mathbf{i}_2 \mathbf{i}_3 \) is the volume of the fundamental cell. The various inverse lattice sites are at \( \mathbf{y}_n = 2\pi n \mathbf{i}_i \mathbf{i}_i \), \( n_i \) integral.
THE GREEN'S FUNCTIONS

Definition of Green's functions.

Among the various techniques now available for discussing normal Fermion systems, probably the most elegant is the use of Green's functions. A correlation or Green's function is the expectation value of a time ordered set of Heisenberg field operators, usually taken in the fully interacting ground state of the many body system. By definition, the one-particle electron and the one-particle positron Green's functions are respectively

\[ G_e(x', x) = \langle i < \tau \psi(x) \psi^+(x') | > \]

and

\[ G_p(x', x) = \langle i < \tau \phi(x) \phi^+(x') | > \]

where \[ | > \] is the ground state of the system and \( \tau \) is the Wick time ordering operator. Similarly, the two particle electron-positron correlation function is by definition

\[ G_{ep}(x, y; x', y') = \langle i < \tau \psi(x) \phi(y) \phi^+(y') \psi^+(x') | > \]

Higher order Green's functions are defined as obvious generalizations of these.

Reasons for introducing such entities.

The advantages of introducing such entities are first that a perturbation expansion for an arbitrary Green's function can be systematically constructed and represented by a set of Feynman graphs, and second that the ground state expectation value of an observable of interest can usually be calculated from a knowledge
of these correlation functions according to a relatively simple prescription. For instance, it will be shown in the next chapter that the total annihilation rate $Q$ (with emission of two quanta) for a system of $W$ electrons and one positron, in their ground state $|W\rangle$, is simply given by an integral over all of space of the electron-positron propagator $G_{ep}(\mathbf{x}, \mathbf{x'}; \mathbf{y}, \mathbf{y'})$. That is, to within a proportionality constant,

$$Q \propto \int d^{3}x' \langle W | \psi(x') \psi(x) \phi^{+}(x') \phi(x) | W \rangle.$$  \hspace{1cm} (3-22)

In order to set up the perturbation series for a given propagator, one first derives the equation of motion for the propagator and then one solves this equation by making a perturbation expansion in powers of the two-body potential $\varphi(y; y')$. It must be stressed, from the very beginning, that this approach is based entirely on the assumption that we are dealing with a normal Fermion system, i.e. one which admits of such a perturbation expansion. This assumption can be considered a basic limitation of our whole calculation.

**Equation of motion for the one-particle propagator.**

Before giving the derivation of the integral-differential equation satisfied by the most general n-body Green's function, it is instructive to first look at the simplest case, namely the one-particle positron propagator. By definition, this Green's function is

$$G_{p}(\mathbf{x}; \mathbf{x'}) = \langle \mathbf{x} | \mathbf{1} \phi(\mathbf{x}) \phi^{+}(\mathbf{x'}) \rangle >$$  \hspace{1cm} (3-13)
Differentiating both sides with respect to the time variable $\gamma$ gives

$$i \partial_{\gamma} \phi(\gamma) = i \left\langle 1 \right| \mathcal{L} \phi(\gamma) \phi(\gamma) \left| 1 \right\rangle - \mathcal{S}^{+}(\gamma, \gamma') \left\langle 1 \right| \mathcal{L} \phi(\gamma) \phi(\gamma') \left| 1 \right\rangle \right. \tag{1-17}$$

where use was made of the anticommutation rules (1-2). The equation of motion for the positron field is

$$i \partial_{\gamma} \phi(\gamma) = \left[ \phi(\gamma), \mathcal{H} \right]. \tag{1-15}$$

Again by reference to the anticommutation rules (1-2) and the definition of the Hamiltonian, the right hand side of (1-15) can readily be evaluated. A little algebra yields

$$i \partial_{\gamma} \phi(\gamma, \gamma') = \mathcal{L} \phi(\gamma, \gamma')$$

$$+ \left[ i \left\langle 1 \right| \mathcal{L} \phi(\gamma, \gamma') \phi(\gamma, \gamma') \left| 1 \right\rangle - \mathcal{S}^{+}(\gamma, \gamma') \left\langle 1 \right| \mathcal{L} \phi(\gamma, \gamma') \phi(\gamma, \gamma') \left| 1 \right\rangle \right. \tag{1-16}$$

Substituting (1-16) into (1-15) gives

$$i \partial_{\gamma} \phi(\gamma, \gamma') = - \mathcal{S}^{+}(\gamma, \gamma') + \mathcal{L} \phi(\gamma, \gamma')$$

$$+ \left[ i \left\langle 1 \right| \mathcal{L} \phi(\gamma, \gamma') \phi(\gamma, \gamma') \left| 1 \right\rangle - \mathcal{S}^{+}(\gamma, \gamma') \left\langle 1 \right| \mathcal{L} \phi(\gamma, \gamma') \phi(\gamma, \gamma') \left| 1 \right\rangle \right. \tag{1-17}$$

The plus signs in $\phi(\gamma, \gamma')$ and $\psi(\gamma, \gamma')$ are introduced to avoid the ambiguity which occurs in a time ordering when a pair of conjugate field operators have the same time variable. Since inside a time ordering operators can be anticommuted at will provided we intro-
duce a \((-1)\) for each such anticommutator, the last term on the
right hand side of (1-17) can be rewritten as

\[ (-i \partial_x + \mathcal{H}_p(x)) G_p(x; x') = \mathcal{S}^i(y-x') \]

\[ -i \left[ \delta_x^3 \nu(x; y) \left[ G_{pp}(3 y; x; 3 x'; x') - G_{pp}(3 y; x; 3 x'; x') \right] \right] . \]  

(1-18)

This is an integral-differential equation for the one-positron
propagator. Note that the positron propagator is coupled through
this equation to the two-particle positron-positron and electron-
positron Green's functions. This coupling is due to the inter-
action between the particles. Indeed, if the two-body potential
\( \nu(x; y) \) vanished, equation (1-9) would simply reduce to

\[ (-i \partial_y + \mathcal{H}_e(y)) G^o_e(y; y') = \mathcal{S}^i(y-x') \]

(1-19)

where the superscript \(^o\) refers to the limit \( \nu(x; y) \to 0 \). By sym-
metry, the one-particle electron propagator satisfies the
equation

\[ (-i \partial_y + \mathcal{H}_e(y)) G_e(y; y') = \mathcal{S}^d(y-x') \]

(1-20)

\[ -i \left[ \delta_x^3 \nu(y; y) \left[ G_{ee}(3 y; x; 3 x'; x') - G_{ee}(3 y; x; 3 x'; x') \right] \right] . \]

Equations (1-18) and (1-20) are the first of an infinite set of
coupled integral-differential equations connecting a given Green's
function to other propagators involving both smaller and greater
numbers of particles. In fact, it is possible to write down the
explicit equation satisfied by an arbitrary Green's function.
The derivation of this equation differs from that of the one-posit-
tron propagator only in added complexity.
Equation of motion for the general Green's functions.

We begin by writing the most general n'th order correlation function as

\[
G_{\alpha_1,\ldots,\alpha_m,\gamma_1,\ldots,\gamma_n} = \int \mathcal{T} \left( \psi_{\alpha_1}(x_1) \cdots \psi_{\alpha_m}(x_m)^\dagger \cdots \psi_{\gamma_1}'(x'_1) \cdots \psi_{\gamma_n}'(x'_n) \right) \]

(1-22)

where \( \alpha_i \) is "e" ("p") if the \( i \)'th field operator appearing in the propagator is the electron (positron) field operator \( \psi(x_i) \) (\( \psi^\dagger(x_i) \)).

Taking the first derivative of (1-21) with respect to the time variable \( \gamma_{i_0} \) leads us to consider the expression

\[
\Gamma_{\gamma_{i_0}} \left( \mathcal{T} \{ \psi_{\alpha_1}(x_1)^\dagger \cdots \psi_{\alpha_m}(x_m)^\dagger \cdots \psi_{\gamma_1}'(x'_1)^\dagger \cdots \psi_{\gamma_n}'(x'_n)^\dagger \} \right)
\]

(1-21)

which can be worked out to be

\[
\mathcal{T} \left( \partial_{\gamma_{i_0}} \psi_{\alpha_1}(x_1) \cdots \psi_{\alpha_m}(x_m)^\dagger \cdots \psi_{\gamma_1}'(x'_1) \cdots \psi_{\gamma_n}'(x'_n) \right)
\]

\[
+ \sum_{j=1}^{n} \left( -1 \right)^{m-1} \delta'(\gamma_{i_0} - \gamma_j) \mathcal{T} \left( \psi_{\alpha_1}(x_1)^\dagger \cdots \psi_{\alpha_m}(x_m)^\dagger \cdots \psi_{\gamma_1}'(x'_1)^\dagger \cdots \psi_{\gamma_j}'(x'_j)^\dagger \cdots \psi_{\gamma_n}'(x'_n)^\dagger \right)
\]

(1-23)

where \( \sum \) means that we are to sum only over the primed electron (positron) co-ordinates if \( \alpha_i \) is an electron (positron) index. To verify that expressions (1-22) and (1-23) are equal, it is perhaps simplest to take the indefinite integral of both (1-22) and (1-23) with respect to \( \gamma_{i_0} \) and check that the two results are identical for arbitrary \( \gamma_{i_0} \).

The equation of motion for the field operator \( \psi_{\alpha_1}(x_1) \) is

\[
\partial_{\gamma_{i_0}} \psi_{\alpha_1}(x_1) = \mathcal{H}_{\alpha_1}(x_1) \psi_{\alpha_1}(x_1)
\]

\[
\mathcal{T} \left[ \delta^2 \mathcal{V}(x_1, x_2) \left( \psi_{\alpha_1}^\dagger(x_1, x_2) \psi_{\alpha_1}(x_2, x_3) - \psi_{\alpha_1}(x_1, x_2)^\dagger \psi_{\alpha_1}(x_2, x_3)^\dagger \right) \right] \psi_{\alpha_1}(x_3, x_4)
\]

(5-24)
where \( x_i' \) stands for "c" ("f") if \( x_i \) is "p" ("e"). Introducing (1-24) into the first term of (1-23), rearranging the field operators in the time ordering, and taking the expectation value of both (1-22) and (1-23) leads to the equality

\[
(-i)^{n-1} \int \frac{d^3 \mathbf{r}}{(2\pi)^3} \left( \frac{\hbar}{\mathbf{i}} \right) G_{a_1, \ldots, a_n} (x_1; \ldots, x_n; x_1', \ldots, x_n')
\]

\[
-\int \frac{d^3 \mathbf{r}}{(2\pi)^3} \left( \frac{\hbar}{\mathbf{i}} \right) \left( \frac{2}{\pi} \right)^{n/2} \exp \left( \frac{\mathbf{r} \cdot \mathbf{r}}{2} \right) G_{a_1, \ldots, a_n} (x_1, \ldots, x_n; x_1', \ldots, x_n') \right]
\]

\[
\sum_{\ii} (-i)^{\ii} \int \frac{d^3 \mathbf{r}}{(2\pi)^3} \left( \frac{\hbar}{\mathbf{i}} \right) G_{a_1, \ldots, a_n} (x_1; \ldots, x_n; x_1', \ldots, x_n')
\]

where for convenience \( G_{a_1, \ldots, a_n} (x_1; \ldots, x_n; x_1', \ldots, x_n') \) stands for

\[
(i)^{n-1} \langle \left| \left[ \Psi_{a_1} (x_1) \right] \ldots \Psi_{a_n} (x_n) \Psi_{a_1}^+ (x_1') \ldots \Psi_{a_n}^+ (x_n') \right| \rangle
\]

Expression (1-26) is of course a Green's function and could be put into the condensed notational form (1-21), but we prefer not to do so. As it stands, the infinite set of equations (1-25) is very general. For instance, the expectation value of the operator

\[
\left\{ \Psi_{a_1} (x_1) \ldots \Psi_{a_n} (x_n) \Psi_{a_1}^+ (x_1') \ldots \Psi_{a_n}^+ (x_n') \right\}
\]

taken in an arbitrary state satisfies this equation. In order to single out the solution appropriate to a system of \( N \) electrons and one positron in their ground state, a boundary condition must be added. The correct boundary condition to be imposed will become clear as we proceed with the solution of the set (1-25).
Change to pure integral equations.

For every equation of the set (1-25) there exists a conjugate equation. The simplest of these will be sufficient for our purpose. In the limit of no two-body interaction, the conjugate equation satisfied by the one-particle Green's function is

\[(i\partial_{\nu} + H_{\alpha}(\nu)) G_{\alpha}^{\star}(\nu;\nu) = \delta^{\star}(\nu - \nu) \quad (1-27)\]

The validity of the equation is obvious. To change the set of equations (1-25), which are integral-differential equations, to a set of purely integral equations, multiply (1-25) on the right by \(G_{\alpha}(\nu;\nu)\) and (1-27) by \(G_{\alpha}^{\star} a_{m}(\nu, \nu_{1} \ldots \nu_{m} ; \nu)\); then subtract the two and integrate over \(d\nu\). This leads to

\[
G_{\alpha} a_{m}(\nu_{1} \ldots \nu_{m} ; \nu_{1} \ldots \nu_{m}^{\prime}) = \sum_{j=1}^{n} \int_{\nu_{j} = \nu_{j}^{\prime}} (\nu_{j} - \nu_{j}^{\prime}) \frac{\partial}{\partial \nu_{j}} G_{\alpha}(\nu_{j} ; \nu_{j}^{\prime}) G_{\alpha}^{\star} a_{m}(\nu_{1} \ldots \nu_{m} ; \nu_{1}^{\prime} \ldots \nu_{m}^{\prime})
\]

\[-i \int d\nu_{1} d\nu_{2} \varphi(\nu_{1}, \nu_{2}) G_{\alpha}(\nu_{1} ; \nu_{2}) \left[ G_{\alpha} a_{m}(\nu_{1}, \nu_{2} \ldots \nu_{m} ; \nu_{1} \ldots \nu_{m}^{\prime}) \right.]

\[- \left. G_{\alpha}^{\star} a_{m}(\nu_{1}, \nu_{2} \ldots \nu_{m}, \nu_{1}^{\prime} \ldots \nu_{m}^{\prime}) \right]\quad (1-28)

where we made use of the fact that

\[
\int d\nu \left[ G_{\alpha}^{\star}(\nu;\nu) \left( -i \frac{\partial}{\partial \nu} + H_{\alpha}(\nu) \right) G_{\alpha}^{\star} a_{m}(\nu, \nu_{1} \ldots \nu_{m} ; \nu_{1} \ldots \nu_{m}^{\prime}) \right]

\[- G_{\alpha} a_{m}(\nu, \nu_{1} \ldots \nu_{m}, \nu_{1} \ldots \nu_{m}^{\prime}) \left( i \frac{\partial}{\partial \nu} + H_{\alpha}(\nu) \right) G_{\alpha}^{\star}(\nu;\nu) \right]\quad (1-29)

vanishes, as can be verified using integration by parts on the second term of (1-29).

A few special cases.

To see how a formal solution of the equations (1-28) can be
constructed systematically in perturbation theory, we can write down a few particular cases of (1-28). The positron propagator satisfies

$$G_\gamma(x; x') = C_\gamma(x; x') - i \int \frac{d^3 p}{(2\pi)^3} \sigma(x; x') G_\gamma(p) \left[ C_{\gamma p}(p, p'; x, x') - C_{\gamma p}(p, p'; x', x') \right] .$$  

(3-20)

The two-body electron-positron and positron-positron correlation functions obey respectively

$$G_{ep}(x, x'; x', x') = C_{ep}(x, x') + G_\gamma(x; x')$$

$$-i \int \frac{d^3 p}{(2\pi)^3} \sigma(x; x') C_{\gamma p}(p) \left[ G_{ep}(p, p'; x, x') - G_{ep}(p, p'; x', x') \right]$$  

(3-31)

and

$$G_{pp}(x, x'; x', x') = C_{pp}(x, x') + G_\gamma(x; x')$$

$$-i \int \frac{d^3 p}{(2\pi)^3} \sigma(x; x') C_{\gamma p}(p) \left[ G_{pp}(p, p'; x, x') - G_{pp}(p, p'; x', x') \right] .$$  

(3-32)

To get $G_\gamma(x, x')$ to first order, $C_{pp}(x, x')$ and $G_{ep}(x, x', x', x')$ are needed to zeroth order. But from (1-31) and (1-32) these are respectively

$$C_{pp}(x, x') G_\gamma(x; x') - C_{pp}(x, x') G_\gamma(x; x')$$

$$C_{ep}(x, x') G_\gamma(x; x') - C_{ep}(x, x') G_\gamma(x; x') .$$  

(3-33)

Hence to first order

$$G_\gamma(x; x') = C_\gamma(x; x') - i \int \frac{d^3 p}{(2\pi)^3} C_\gamma(x; p) \sigma(p; x') \left[ C_\gamma(p, p'; x, x') - C_\gamma(p, p'; x', x') \right] - C_\gamma(x, x') C_\gamma(x, x') .$$  

(3-34)
Feynman graphs representing the four terms in (1-31) are shown in figure 1-1. If the positron propagator is required to second order, we need to know both $G_{\gamma\gamma}$ and $G_{\gamma\gamma}$ to first order, which in turn requires a knowledge of $G_{\gamma\gamma}$, $G_{\gamma\gamma}$, $G_{\gamma\gamma}$, and $G_{\gamma\gamma}$ to zeroth order, which we have. The construction of the positron propagator to any order is then clear, although it may become quite tedious.

**Figure 1-1**

(a)  (b)  (c)  (d)

Positron propagator to first order.

The function which is central to this thesis is not the positron propagator but the electron-positron correlation function. To obtain this function to first order, it is evident from (1-31) that a knowledge of $G_{\gamma\gamma}$ and $G_{\gamma\gamma}$ to zeroth order is sufficient. But from equation (1-28) these are respectively

\[ G_{\gamma\gamma}(x, y, \xi, \eta; x', y', \xi', \eta') = G_{\gamma}(x, y; x', y') G_{\gamma}(\xi, \eta; \xi', \eta') - G_{\gamma}(\xi, \eta; x', y') G_{\gamma}(x, y; \xi', \eta') \]

and

\[ G_{\gamma\gamma}(x, y, \xi, \eta; x', y', \xi', \eta') = G_{\gamma}(x, y; x', y') G_{\gamma}(\xi, \eta; \xi', \eta') - G_{\gamma}(\xi, \eta; x', y') G_{\gamma}(x, y; \xi', \eta'). \]

Substituting (1-35) into (1-31), it becomes to first order
The graphical representation of (1-36) is given in figure 1-2. The doubled wavy line in graph 1-2a represents the positron propagator to first order as given in figure 1-1. Each graph in figures 1-1 and 1-2 represents a perturbation term in the series for a given Green's function. It is possible to set up rules which enable one to write down explicitly the contribution to

Figure 1-2

Electron-positron propagator to first order. The double wavy line in (e) stands for the positron propagator to first order.
the Green’s function from any such diagram. These rules can in fact be deduced from formulae (1-34) and (1-36).

Feynman rules.

To write down the perturbation term represented by a given Feynman graph, apply the following prescription:

1). For each electron line \( \gamma_i \) to \( \gamma_f \) write \( G_e(\gamma_i;\gamma_f) \).

2). For each positron line \( \gamma_i \) to \( \gamma_f \) write \( G_p(\gamma_i;\gamma_f) \).

3). For each instantaneous coulomb interaction line \( \gamma_i \) to \( \gamma_f \) write \( i(\gamma_i;\gamma_f) \).

4). Write an overall sign factor \( (-1)^{\lambda+1} \), where \( \lambda \) is the number of closed loops appearing in the graph and \( \lambda' \) is the number of electron-positron interactions.

For a complete specification of the perturbation series by Feynman graphs and rules, it is necessary to add to the four rules given above a new set for the construction of all acceptable (topologically different) diagrams in a given order. This is more difficult and certainly cannot be deduced in an unambiguous way from the graphs of figures 1-1 and 1-2. To get an idea of what these should be, the electron-positron propagator was worked out to second order. Writing down all of the sixty nine terms which arise would be quite useless; instead, forty of the terms are given graphically in figure 1-3. Diagrams 1 to 21 can be described as second order electron self energy processes with an added free positron line (unlinked). From these, 21 new diagrams can be
Figure 1-3: Forty second order diagrams in the expansion of the electron-positron propagator.
generated by replacing all electron (positron) lines by positron (electron) lines. The resulting graphs are the positron self energy processes. Diagrams 22 to 39 are all linked diagrams, each involving one or no self energy part. This gives a total of sixty terms. The last diagram is one of the remaining nine terms which give the expansion of \( G_e^{(l)}(\eta; \eta ') G_p^{(l)}(\xi; \xi ') \). They are unlinked, with one electron and one positron self energy part. Clearly, to second order the electron-positron propagator can be written as

\[
G_{eq}^{(l)}(\eta; \eta ') G_p^{(l)}(\xi; \xi ') = G_e^{(l)}(\eta; \eta ') G_p^{(l)}(\xi; \xi ') + G_e^{(l)}(\eta; \eta ') G_p^{(l)}(\xi; \xi ') + F_{eq}(\eta; \eta ') G_p^{(l)}(\xi; \xi ') + F_{eq}(\eta; \eta ') G_p^{(l)}(\xi; \xi ')
\]

with \( F_{eq}(\eta; \eta ') G_p^{(l)}(\xi; \xi ') \) defined as the sum of graphs 22 to 39. With the help of figure 1-3 it is not difficult to formulate general rules for drawing all \( n \)th order diagrams in the expansion of the electron-positron propagator. These rules turn out to be so similar to the well known rules for an electron gas that we will not bother writing them down. Furthermore, the diagrams of figures 1-1, 1-2, and 1-3 are sufficient for our purposes in this thesis.

Boundary conditions.

The basic constituents of the perturbation series for an arbitrary Green's function are the free electron propagator \( G_e(\eta; \eta ') \), the free positron propagator \( G_p(\xi; \xi ') \), and the two-body potential \( \Sigma(\eta; \eta ') \). It is clear that the boundary conditions to be imposed in order to single out the solution of (1-28) appropriate to a system of \( N \) electrons and one positron in their ground state |\( N_1 \rangle \).
must reduce to boundary conditions on \( G^r_\varepsilon(x',x') \) and \( G^s_\varepsilon(x',x') \). These two functions will now be studied in detail. The free positron propagator satisfies equation (1-19). When the lattice potential is included, the system is not invariant under an arbitrary displacement, but it still exhibits the weaker symmetry of invariance under translation through a primitive lattice vector \( \mathbf{y}_c \). Hence

\[
G^r_\varepsilon(\mathbf{x}_1,\mathbf{y}_c; \mathbf{x}_1',\mathbf{y}_c') = G^r_\varepsilon(x,x') \quad \text{for arbitrary } x, x'.
\]

From (1-39) it is concluded that the positron propagator can be written in the form

\[
G^r_\varepsilon(x,x') = \left( \begin{array}{c}
\mathbf{y}_c \\
\mathbf{y}_c'
\end{array} \right) \mathbf{n}_{\mathbf{k}^\mathbf{A}} \mathbf{n}_{\mathbf{k}^\mathbf{A}'} \left( \mathbf{q} \right) \mathbf{n}_{\mathbf{k}^\mathbf{A}} \mathbf{n}_{\mathbf{k}^\mathbf{A}'} \left( \mathbf{q} \right) \left( \begin{array}{c}
\mathbf{y}_c \\
\mathbf{y}_c'
\end{array} \right) \mathbf{G}_{\mathbf{k}^\mathbf{A}} \left( \mathbf{k}^\mathbf{A} ; \omega \right),
\]

where use was made of the invariance of the theory under an arbitrary displacement of the time origin. The functions \( \mathbf{n}_{\mathbf{k}^\mathbf{A}} \) and \( \mathbf{n}_{\mathbf{k}^\mathbf{A}'} \) are the Bloch states for the positron, \( \mathbf{k}^\mathbf{A} \) is the crystal momentum restricted to the first Brillouin zone, and \( \lambda (\mathbf{q}^\prime) \) is a band index. Inserting (1-39) into equation (1-19) gives

\[
(-\omega - E^p_{\mathbf{k}^\mathbf{A}}) \mathbf{G}_{\mathbf{k}^\mathbf{A}} \left( \mathbf{k}^\mathbf{A} ; \omega \right) = \mathbf{S}_{\mathbf{k}^\mathbf{A}}
\]

where \( E^p_{\mathbf{k}^\mathbf{A}} \) is the energy of the Bloch state \( \mathbf{y}_c \mathbf{n}_{\mathbf{k}^\mathbf{A}} \left( \mathbf{q} \right) \). From (1-40) it is evident that only one band index is needed to specify the "Fourier transform" of the free positron propagator. This can be taken advantage of to introduce a simplified notation for \( \mathbf{G}_{\mathbf{k}^\mathbf{A}} \left( \mathbf{k}^\mathbf{A} ; \omega \right) \).

Write

\[
\mathbf{G}_{\mathbf{k}^\mathbf{A}} \left( \mathbf{k}^\mathbf{A} ; \omega \right) = \left( \begin{array}{c}
\mathbf{y}_c \\
\mathbf{y}_c'
\end{array} \right) \mathbf{n}_{\mathbf{k}^\mathbf{A}} \mathbf{n}_{\mathbf{k}^\mathbf{A}'} \left( \mathbf{q} \right) \mathbf{n}_{\mathbf{k}^\mathbf{A}} \mathbf{n}_{\mathbf{k}^\mathbf{A}'} \left( \mathbf{q} \right) \left( \begin{array}{c}
\mathbf{y}_c \\
\mathbf{y}_c'
\end{array} \right) \mathbf{G}_{\mathbf{k}^\mathbf{A}} \left( \mathbf{k}^\mathbf{A} ; \omega \right)
\]
with
\[ G_{\text{pa}}(k', \omega) = \frac{1}{(E_{k,k}^e - \omega)}. \] (1-42)

When a path of integration is specified for the \( \omega \) variable the positron propagator is completely determined. Clearly the boundary condition to be imposed on the solution of the set of equations (1-25) is now reduced to the problem of choosing an appropriate contour in the complex \( \omega \)-plane. Tentatively choose a path extending from \( -\infty \) to \( E_{\text{lo}}^e \) (the lowest Bloch energy for a positron in the crystal field \( V_p(\mathbf{r}) \)) just below the real axis, crossing at the point \( E_{\text{lo}}^e \) and extending to \( \infty \) just above the axis. Equivalently, choose as path the real \( \omega \)-axis and change (1-42) to
\[ G_{\text{pa}}(k', \omega) = \frac{\Theta^0(-\kappa)}{E_{k,k}^e - \omega + i\gamma} + \frac{\Theta^\nu(\kappa)}{E_{k,k}^e - \omega - i\gamma}, \] (1-43)

where by definition
\[ \Theta^0(-\kappa) = 0 \quad \text{for} \quad l \neq 0 \neq \kappa \]
\[ = 1 \quad \text{for} \quad l = 0 \neq \kappa \]
\[ \Theta^\nu(\kappa) = 1 \quad \text{for} \quad l \neq 0 \neq \kappa \]
\[ = 0 \quad \text{for} \quad l = 0 \neq \kappa. \]

The specification of the positron propagator is now complete. For \( t-t' > 0 \) (\( t-t' < 0 \)) the contour in (1-41) is closed below (above) giving
\[ G_{\text{f}}(k', k) = \frac{-i}{V} \sum_{(k), \neq 0} \frac{\delta_{k}(k') \delta_{k}(k')}{E_{k,k}^{\text{lo}}(k') \omega_{k,k}^{\text{lo}}(k')} e^{-iE_{k,k}^e(t-t')} \quad t-t' > 0 \] (1-44)
\[ = \frac{-i}{V} \sum_{(k), \neq 0} \frac{\delta_{k}(k') \delta_{k}(k')}{E_{k,k}^{\text{lo}}(k') \omega_{k,k}^{\text{lo}}(k')} e^{-iE_{k,k}^e(t-t')} \quad t-t' < 0 \]
To verify that our choice of contour was correct, the free positron propagator for a system of $N$ free electrons and a free positron in their ground state can be evaluated directly from its definition (1-10). Introducing the Fourier decomposition (1-5) of the field operators in (1-10) taken in the limit of no interactions immediately yields (1-44).

The free electron propagator $G_e(x;x')$ can be handled in a similar fashion. Its Fourier transform takes the form

$$
G_e^{ikl}(k';k) = \frac{\Theta^{ikl}(k'-k)}{E_k^e - \omega + i\eta} + \frac{\Theta^{ikl}(k-k')}{E_{k'}^e - \omega - i\eta},
$$

where by definition

$$
\Theta^{ikl}(k'=k) = 0 \text{ for } (k1) > (l_f k_f) \quad \text{i.e. unoccupied states}
$$

$$
\Theta^{ikl}(k'-k) = 1 \text{ for } (k1) \leq (l_f k_f) \quad \text{i.e. occupied states}
$$

Using (1-45) it is easy to verify that

$$
G_e^{ikl}(k';k) = \sum_{(k1) > (l_f k_f)} \frac{i \Gamma^{ikl}(k'-k)}{V(k1) > (l_f k_f)} U_{kl}^e(k) U_{kl}^e(k') a_c^{E_k^e (1-t\gamma)} \quad t - \gamma > 0
$$

$$
= \sum_{(k1) \leq (l_f k_f)} \frac{i \Gamma^{ikl}(k'-k)}{V(k1) < (l_f k_f)} U_{kl}^e(k) U_{kl}^e(k') a_c^{E_k^e (1-t\gamma)} \quad t - \gamma < 0
$$

The perturbation series for the electron-positron correlation function is now completely specified.
Chapter 2

FORMAL THEORY OF ANNIHILATION

Fundamental formula for the annihilation rate.

To describe the annihilation process, it is of course necessary to use quantum electrodynamics. The detailed reduction of the appropriate S-matrix element will not be given here. R.A. Ferrell, in his 1956 review article, has given a very simple discussion of this problem taking advantage of the considerable simplification introduced when one is concerned only with very low energy particles. This is certainly the case in positron annihilation experiments where the positron is thermalized on annihilation, and where a typical valence electron energy is of the order of a Rydberg. In the language of Green's functions, Ferrell's result for the partial annihilation rate \( \mathcal{G}_p \) with emission of a photon pair of total momentum \( \mathbf{p} \) is, to within a proportionality constant,

\[
\mathcal{G}_p \propto \frac{\omega^2}{\mathcal{V}} \int d^3\mathbf{q} \, \Delta_{\text{ep}}(\mathbf{x}; \mathbf{q}, \mathbf{q}^\ast, \mathbf{q}^\ast) \, d^3\mathbf{q} \, d^3\mathbf{q}^\ast.
\]

Recalling the definition of the two-particle electron-positron propagator (1-11), the expression (2-1) can be rewritten in perhaps a more familiar form:

\[
\mathcal{G}_p \propto \left\langle \Psi(\text{\emph{W}4}) \, \frac{1}{\mathcal{V}} \int d^3\phi^\ast \phi^\dagger(\mathbf{x}) \phi^\dagger(\mathbf{y}) \, d^3\phi \right\rangle \left\langle \phi(\mathbf{x}^\ast) \phi(\mathbf{y}^\ast) \, d^3\phi \right\rangle
\]

where \( \Psi(\text{\emph{W}4}) \) is the fully interacting Heisenberg ground state of a system of \( N \) electrons and a positron. The quantities \( \Psi(\mathbf{x}) \) and \( \phi(\mathbf{x}) \) are respectively the electron and positron field operators.
as defined in Chapter 1. To get the total annihilation rate $Q$ from (2-2) it is only necessary to sum over all possible momenta $\hat{q}$ for the emitted photon pair, i.e. $Q = \sum_{\hat{q}} Q_{\hat{q}} \propto m$ where, by definition

$$m = \int d^3x \left\langle V_{\text{1A}} \psi^*(x) \psi(x) \phi^*(x) \phi(x) \right\rangle.$$

As introduced, $m$ is the electron density at the positron position, averaged over all positron positions. The proportionality constant in (2-1) and (2-3) can conveniently be fixed by reference to the known properties of singlet positronium. The electron density at the positron in the positronium ground state is $\sqrt{2}n_0$, and the annihilation rate is $4\lambda_0$ with $\lambda_0 \approx 2.6 \times 10^4 \text{sec}^{-1}$. Hence

$$Q_{\text{positronium}} = 4\lambda_0 \sqrt{2} n_0 \propto n_{\text{positronium}}.$$ Since annihilation into two quanta can only occur from a singlet spin state $^{1S}$, the correct proportionality constant for a metal is $4\lambda_0 \sqrt{2} n_0 \frac{1}{4}$. The factor $\frac{1}{4}$ is just the probability for a given electron-positron pair in a metal to be in a singlet state. Hence $Q = \lambda_0 m$ and

$$Q_{\hat{q}} = \lambda_0 \left(\frac{1}{4}\right)^3 \int \frac{d^3p}{V} \frac{d^3\xi}{V} \frac{d^3\alpha}{V} \frac{d^3\beta}{V} \frac{d^3\gamma}{V} \left\langle \xi \phi \phi \psi \right\rangle \left\langle \alpha \beta \gamma \right\rangle \left\langle \psi \phi \phi \right\rangle \left\langle \xi \phi \phi \psi \right\rangle$$

where for convenience $\lambda$ has been introduced to denote $\lambda_0 \sqrt{2} n_0$. Formula (2-4) is basic to this thesis. The remaining chapters will deal exclusively with the evaluation of $Q_{\hat{q}}$ and $Q$ for various metals. This clearly reduces to making some approximate estimate of the two-body electron-positron correlation function appropriate to the particular metal under consideration.

**Sommerfeld model**

As a first application of equation (2-4), consider the case in which all interactions are neglected. The simple picture that
results is called the Sommerfeld model. This is a considerable simplification of an actual metal but it is known to be a very good first approximation to many metals, sodium for instance. In the limit of no interaction, the electron-positron Green's function \( G_{\gamma} (\mathbf{q}, \mathbf{q}; \mathbf{q}^+, \mathbf{q}^+) \) reduces to \( G_{\gamma} (\mathbf{q}^+) G_{\gamma} (\mathbf{q}^+) \). The positron propagator \( G_{\gamma} (\mathbf{q}^+) \) and the electron propagator \( G_{\gamma} (\mathbf{q}^+) \) are given respectively by (1-44) and (1-46) taken in the limit of no lattice. For the particular argument \((\mathbf{q}, \mathbf{q}^+)\) this gives \( G_{\gamma} (\mathbf{q}, \mathbf{q}^+) = \mathbf{i} \sum_{\mathbf{q}^+} G_{\gamma} (\mathbf{q}^+) \). (Note that in this approximation the thermalized positron is at rest and distributed with a uniform probability throughout the metal.) Hence for this model the annihilation rate into a two-photon pair of total momentum \( \mathbf{q} \) is

\[
\dot{\rho}_{\mathbf{q}} = \lambda \cdot 2 \cdot \frac{1}{V} \sum_{\mathbf{k}, \mathbf{k}_{\mathbf{p}}} \delta_{\mathbf{k}, \mathbf{q}}
\]

The factor of 2 enters because of spin degeneracy. As it stands, formula (2-5) is not very useful since \( \dot{\rho}_{\mathbf{q}} \) is not readily measurable experimentally. The quantity that is measured in the usual angular correlation experiment is rather the number of photon pairs having a component of total momentum \( \mathbf{p}_3 \) in some fixed direction. (taken to be the \( \mathbf{z} \)-direction). That is, to within a proportionality constant, one measures the distribution function for the \( \mathbf{z} \)-component of momentum :

\[
\dot{\rho}_{\mathbf{p}_3} = \sum_{\mathbf{p}_3} \dot{\rho}_{\mathbf{q}} = \lambda \cdot 2 \cdot \frac{1}{V} \sum_{\mathbf{k}, \mathbf{k}_{\mathbf{p}}} \delta_{\mathbf{k}, \mathbf{q}}
\]

A typical experimental arrangement is shown schematically in figure 2-1. When the total momentum of the photon pair is zero they come out "back to back," each with energy \( mc^2 \). On the other hand, when \( \mathbf{q} \) is not zero, they no longer emerge at an angle of \( \pi \) radians but rather at a slightly smaller angle \( \pi - \alpha \). It is clear
A possible experimental set-up for an angular correlation experiment. Two detectors are operated in coincidence, one fixed and shielded, the other moving in the $y$-$z$ plane on the arc of a circle centered at the source. As positron source one could use an Na$^+$ sample and wrap the material to be studied around it.

From figure 2-1 that what is measured is not the number of photons coming out at an angle $\alpha$, but rather the number with projection of $\alpha$ in the $y$-$z$ plane equal to $\theta$, the angle between the two planes defined by the detector slits and the source. This angle is simply related to the component of total momentum of the pair in the $z$-direction. Because $\mathbf{p}$ is necessarily small compared to $mc$, we get $\theta = \mathbf{p}_z/mc$.

To evaluate the right hand side of equation (2-6), it is convenient to go over to the limit of infinite volume. In this limit all sums go over into integrals and
Because the system is isotropic the integral (2-7) is independent of the actual 3-direction chosen. Let \( \mathbf{\hat{a}} \) be a unit vector in this direction. As \( q \) ranges over the plane \( q \cdot \mathbf{\hat{a}} = 0 \), the delta function \( \delta^2(q - q) \) is zero unless we are inside the Fermi sphere, in which case it has weight 1. So for \( p_d > k_f \), \( \Theta_{f3} \) is zero, and for \( p_d < k_f \) it is just proportional to the area of the circle giving the intersection of the plane \( q \cdot \mathbf{\hat{a}} = q \) with the sphere \( |q| = k_f \).

Hence

\[
\Theta_{f3} = \begin{cases} 0 & \text{for } p_d > k_f \\ \lambda^2 \frac{2\pi}{(2\pi)^3} (k_f^2 - p_d^2) & \text{for } p_d < k_f \\ \end{cases}
\]

Finally, the total annihilation \( \Theta \) is the integral of \( \Theta_{f3} \) taken over all \( p_d \) 's:

\[
\Theta = \int_0^{k_f} \Theta_{f3} \, dp_d = \lambda^2 \frac{2\pi}{(2\pi)^3} \frac{4}{3} k_f^3.
\]

But \( \frac{4}{3} k_f^3 (2/\pi)^3 \) is just the number of valence electrons per unit crystal volume. It is convenient to introduce a dimensionless parameter \( \eta_0 \) to characterize the density \( n_v \) of the electron gas corresponding to a particular metal. By definition \( \eta_0 \) is the radius of a sphere, in Bohr units, which on the average contains one valence electron; i.e.,

\[
\frac{4}{3} \pi k_f^3 (2/\pi)^3 |n_v| = \frac{1}{3} \left( \frac{4}{3} \pi \eta_0^3 \right) \quad \text{or} \quad \eta_0 k_f = \frac{1}{4\pi^2} \eta_0 k_f.
\]

Hence \( \Theta^0 = 6 \lambda \eta_0 k_f^{-3} \), where the superscript \( '0' \) is introduced to indicate that this is the Sommerfeld annihilation rate.

Finally, for comparison with experiment it is useful to change \( p_d \) in (2-8) to the angle \( \Theta (\frac{k_f}{m_c}) \) measured experimentally.
If a cut-off angle $\Theta_c$ is defined by $\Theta_c = \frac{\hbar c}{m c} = 13.99 / a_c$ (milliradians), equation (2-8) can be rewritten as

$$
\phi_{\theta_0} = \begin{cases} 0 & \text{if } \theta > \Theta_c \\ \left( \lambda \cdot \frac{2}{(\pi)^2} \cdot \frac{\pi}{3} k_F^2 \right) \frac{2}{4} k_F \left( 1 - \frac{\theta_c^2}{\theta_0^2} \right) & \text{if } \theta < \Theta_c 
\end{cases}
$$

Next introduce $\phi^0(\theta)$ such that by definition $\phi^0 = \int_{-\infty}^{\infty} d\theta \phi(\theta)$.
Then $\phi^0(\theta)$ is given by

$$
\phi^0(\theta) = \begin{cases} 0 & \text{if } \theta > \Theta_c \\ \phi^0 \cdot \frac{1}{2} \Theta_c \left( 1 - \frac{\Theta_c^2}{\theta_0^2} \right) & \text{if } \theta < \Theta_c 
\end{cases}
$$

The angular correlation curve is therefore an inverted parabola with cut-off at $\Theta_c$, where the curve cuts the $\Theta$-axis. This completes the Sommerfeld theory of positron annihilation in metals.

It is interesting to compare the Sommerfeld theory with experiment. In figure 6-3 the experimental results of A.T. Stewart are given for the angular distribution of the gamma-rays found in sodium. The photon pair counting rate (in arbitrary units) is given as a function of the angle $\Theta$ between the two photons. Except for the broad "tails" at angle greater than $\Theta_c$, the rest of the distribution does not deviate very much from an inverted parabola with cut-off at $\Theta_c$. The broad "tails" beyond $\Theta_c$ do not come from annihilation with the valence electrons, which are the only ones included in the Sommerfeld model. Rather, these tails come from core annihilation as will be shown in Chapter 7. It would seem then that the simple Sommerfeld model has a good deal of validity.

The situation for the total annihilation rates is very
different. In figure 2-2, $\xi$ is plotted against $\eta$, and for comparison the experimental rates found by Bell and Jorgensen\textsuperscript{17} for the alkali metals and aluminium are also shown. The failure of the Sommerfeld model is obvious. Not only does it predict annihilation rates which are much too small for most metals, but also the variation of $\xi$ with $\eta$ is much too large. This failure of the Sommerfeld model may be puzzling at first sight. However it was eventually recognized that what is needed to bring theory and experiment into agreement is not so much a better model of a metal but rather a serious consideration of the annihilating electron-positron coulomb force. This interaction is attractive and should increase considerably the electron density at the positron and hence the annihilation rate. To take this force into account is not simple and only recently (Kahana) was this done in a satisfactory way. Briefly, the difficulty is as follows. If the annihilating electron-positron pair were in free space, then the force between the electron and the positron would be a simple coulomb inverse square law. But the annihilation takes place in a medium, i.e. in the interior of a metal. Clearly the force between annihilating electron and positron must be modified by the presence of all the other valence electrons free to move around in the metal. It is precisely the choice of an adequate effective potential which causes some difficulty. This matter will be considered in detail in the next chapter where Kahana's theory will be discussed. In conclusion, Kahana's theoretical curve is shown in figure 2-2. If one remembers that core annihilation will tend to push the theoretical curve up a little, the agreement with experiment is quite good, at least for metals with density lower than that of aluminium.
Figure 2-2.

Variation of the total annihilation rate with valence electron density. The theoretical curve of Kahana is compared with the experimental work of Bell and Jørgensen. Also shown is the Sommerfeld annihilation rate $\Omega_0 \approx 12 / \sigma_0^2 \times 10^4 \text{sec}^{-1}$. The theoretical point at $n_e = 1.89$ comes from numerical work done in this thesis.
A theorem.

When one wants to go beyond the simple Sommerfeld model there are many different diagrams in the perturbation series to be considered (see Chapter 1). The following theorem is helpful as a guide in sorting these out.

It has already been shown explicitly that to second order (formula 1-37) the electron-positron propagator can be written in the form

\[ G_{\text{ep}}(\mathbf{x}; \mathbf{y}) = G_{\text{e}}(\mathbf{x}; \mathbf{y}) G_{\text{p}}(\mathbf{x}; \mathbf{y}) + F_{\text{ep}}(\mathbf{x}; \mathbf{y}; \mathbf{y}) \]  

with \( G_{\text{e}}(\mathbf{x}; \mathbf{y}) = i \langle \mathcal{N}_1 | \Psi(\mathbf{x}) \Psi^*(\mathbf{y}) | \mathcal{N}_4 \rangle \), \( G_{\text{p}}(\mathbf{x}; \mathbf{y}) = i \langle \mathcal{N}_1 | \Phi(\mathbf{x}) \Phi^*(\mathbf{y}) | \mathcal{N}_4 \rangle \), and \( F_{\text{ep}}(\mathbf{x}; \mathbf{y}; \mathbf{y}) \) is made up of diagrams in which the positron part is connected to the electron part by at least one coulomb interaction line. The validity of (2-11) to all orders is obvious. Consider the case of no crystal potential. If the Fourier decomposition (1-5) of the field operators is introduced into the definition of \( G_{\text{e}}(\mathbf{x}; \mathbf{y}) \) and \( G_{\text{p}}(\mathbf{x}; \mathbf{y}) \), and conservation of momentum is used, we get

\[ G_{\text{e}}(\mathbf{x}; \mathbf{y}) = \frac{i}{\sqrt{\mathcal{N}_4}} \sum_{\mathbf{k}} i^{\mathbf{k} \cdot (\mathbf{x} - \mathbf{y})} \langle \mathcal{N}_1 | a_{\mathbf{k}}^\dagger(\mathbf{y}) a_{\mathbf{k}}(\mathbf{y}) | \mathcal{N}_4 \rangle, \]  

with a similar expression for the positron propagator. But the expectation value on the right hand side of (2-12) is just \( \theta_{\text{e}}(\mathbf{y}) \), the probability of occupation of the state \( |\mathbf{y}\rangle \) by an electron. Thus

\[ G_{\text{e}}(\mathbf{x}; \mathbf{y}) = \frac{i}{\sqrt{\mathcal{N}_4}} \sum_{\mathbf{k}} i^{\mathbf{k} \cdot (\mathbf{x} - \mathbf{y})} \theta_{\text{e}}(\mathbf{y}). \]  

A similar expression holds for the positron:

\[ G_{\text{p}}(\mathbf{x}; \mathbf{y}) = \frac{i}{\sqrt{\mathcal{N}_4}} \sum_{\mathbf{k}} i^{\mathbf{k} \cdot (\mathbf{x} - \mathbf{y})} \theta_{\text{p}}(\mathbf{y}). \]
The contribution from pure self energy diagrams to the partial annihilation rate can then be written as

$$\rho_p = \frac{\lambda}{V} \sum_{\kappa} \frac{p}{e^{\varepsilon_{\kappa} - \mu + \frac{1}{2} \Delta^2}} \rho_e(\kappa) \rho_p(\kappa) = \frac{\lambda}{V} \int \frac{d^3p}{(2\pi)^3} \rho_e(p) \rho_p(p).$$

(2-15)

For an interacting electron gas $\rho_e(\kappa)$ and $\rho_p(\kappa)$ are not simple theta functions and hence the partial annihilation rate is certainly changed from its Sommerfeld value. This is not so for the total annihilation rate. Note that

$$\rho = \sum_{\kappa} \rho_p = \frac{\lambda}{V} \int \frac{d^3p}{(2\pi)^3} \rho_e(p) \rho_p(p) = \lambda \int \frac{d^3p}{(2\pi)^3} \rho_e(p) \rho_p(p).$$

(2-16)

and $\sum_{\kappa} \rho_e(\kappa) = \langle \psi \mid \sum_{\kappa} \rho_e(\kappa) \mid \psi \rangle = \text{number of electrons (spin degeneracy included)}$ while $\sum_{\kappa} \rho_p(\kappa) = 1$. Thus $\rho = \lambda \cdot \eta_v = 1 = \rho^0$. Self energy effects alone cannot change the total annihilation rate. This theorem was first pointed out by Kabana (9).

Another useful observation is the following. Suppose that coulomb interactions are neglected but the lattice potential is included. Then the total annihilation rate $\rho$ is given by

$$\rho = \frac{\lambda}{V} \int \frac{d^3p}{(2\pi)^3} \rho_e(p) \rho_p(p) \rho_v(p),$$

(2-17)

which in general is not $\rho^0$. If however either the positron or electron Bloch states are approximated by a plane waves (for definiteness take the positron function and set $\rho_v(p) = 1$) then

$$\rho = \frac{\lambda}{V} \int \frac{d^3p}{(2\pi)^3} \rho_e(p) \rho_p(p) \rho_v(p) \approx \text{number of electrons} \frac{\lambda}{V} = \rho^0$$

(2-18)

Hence both the electron and positron Bloch states must differ appreciably from plane waves if the total annihilation rate is to be changed from its Sommerfeld value.
Feynman graphs which do not contribute to $\theta_{\mathfrak{f}}$

There is a large number of the diagrams given in figures 1-2 and 1-3 which do not contribute to the partial annihilation rate $\theta_{\mathfrak{f}}$. For simplicity, the lattice potential is neglected (i.e., $V_c=V_p=0$) throughout this section, although most of the results arrived at are not dependent on this assumption. To begin consider diagram 1-2d. It represents the free propagation of a positron while an electron interacts once with the negative charge of the passive electron sea. Its contribution to the electron-positron correlation function $G_e(p, \kappa_i; \kappa'_1, \kappa'_2)$ is

$$G_e(p, \kappa_i; \kappa'_1, \kappa'_2) = \frac{1}{\sqrt{2 \pi \hbar^2}} \int d^{3} \xi \, \langle \psi(\xi, x) | \phi(x) \rangle \langle \phi(x) | \psi(\xi, x) \rangle$$

But $G_e(p, \kappa_i; \kappa'_1, \kappa'_2)$ is the electron part of $G_e(p, \kappa_i; \kappa'_1, \kappa'_2)$ equal to the electron density in the system and $G_e(p, \kappa_i; \kappa'_1, \kappa'_2) = m_e$. Thus, the electron part of (2-19) can be rewritten as

$$G_e(p, \kappa_i; \kappa'_1, \kappa'_2) = \int d^{3} \xi \, m_e \langle \psi(\xi, x) | \phi(x) \rangle \langle \phi(x) | \psi(\xi, x) \rangle$$

On the other hand, by setting $V_c=V_p=0$ we neglect to account for the fixed uniform background of positive charge neutralizing the system, and a correction term of the form

$$\int d^{3} \xi \, m_e \langle \psi(\xi, x) | \phi(x) \rangle \langle \phi(x) | \psi(\xi, x) \rangle$$

should really be added to the Hamiltonian (1-1). Thus the set of coupled integral equations (1-28) should be replaced by the set

$$G_{q_i \cdots q_m} (x_1 \cdots x_n, x'_1 \cdots x'_m) = \sum_{\xi=0}^{m} \int \frac{d^{3} \xi}{(2\pi \hbar^2)^{3/2}} \langle \psi(\xi, x) | \phi(x) \rangle \langle \phi(x) | \psi(\xi, x) \rangle G_{q_i \cdots q_m} (x_1 \cdots x_n, x'_1 \cdots x'_m)$$
Using (2-22) would lead to four first order terms in the perturbation expansion of the electron propagator. They would be the electron part of graphs 1-2b, 1-2c and 1-2d, with the fourth term of the form which is just the negative of (2-20). Thus diagram 1-2d can be dropped. Using (2-22) it is not difficult (but quite tedious) to check that this cancellation remains in higher orders as well. Thus we come to the conclusion that every diagram containing a part ••••• can be dropped since it cancels against the assumed fixed background of positive charge.

The next class of diagrams which we want to consider are those leading to contributions to \( \hat{\varrho}_f \) proportional to the positron density in the system. This density \( n_f \) is equal to \( \gamma \) and in the limit of infinite volume vanishes; hence the contribution to \( \hat{\varrho}_f \) from this diagram also vanishes. Simple examples of members of this class are diagrams containing a loop ••••• or •••••. Perhaps a less trivial example is diagram 1-3 (36) which we will now consider in some detail. First note that it can be derived from 1-3 (39) by simply changing all electron (positron) lines to positron (electron) lines. In Chapter 4 the contribution to \( \hat{\varrho}_f \) from diagram 1-3 (39) is investigated and it is found that it can be written in the form (4-19). Changing all electron (positron) sub-
scripts in (4-19) to positron (electron) subscripts, and using
\( \psi(x; \gamma) \) instead of the static effective potential \( \psi(x; \gamma') \) (to be
defined later) gives the contribution to \( \beta_f \) from 1-3 (36) as

\[
\begin{align*}
\beta_f & = \frac{\lambda(c)^2}{V^3} \sum_{\frac{k}{\beta}} \left[ \frac{d\omega}{2\pi} \psi(x; \omega) \int \frac{d\omega'}{2\pi} G^0_P(k; \omega') G^0_P(k-\frac{e}{\beta}; \omega + \omega') \right] \\
& \text{where} \quad G^0_P(k; \omega) \text{ and } G^0_P(k; \omega') \text{ are given by (1-43) and (1-45) respect­}
\end{align*}
\]

where \( G^0_P(k; \omega) \) and \( G^0_P(k; \omega') \) are given by (1-43) and (1-45) respect­
ively taken in the limit of no lattice potential. But by making
use of (4-20) the integration over \( \omega \) and \( \omega' \) can be performed,
giving four terms:

\[
\begin{align*}
\beta_f & = \frac{\lambda(c)^2}{V^3} \sum_{\frac{k}{\beta}} \left[ \frac{d\omega}{2\pi} \psi(x; \omega) \int \frac{d\omega'}{2\pi} G^0_P(k; \omega') G^0_P(k-\frac{e}{\beta}; \omega + \omega') \right] \\
& \text{where} \quad G^0_P(k; \omega) \text{ and } G^0_P(k; \omega') \text{ are given by (1-43) and (1-45) respect­}
\end{align*}
\]

Each term in (2-25) contains two positron theta functions of the
form \( \Theta(x) \) which can be used to carry out two of the summations.
Thus (2-25) becomes
\[ \Theta_{q} = \frac{2\lambda}{V} \sum_{k} \left[ \frac{d\psi}{d\pi} \frac{d\phi}{d\pi} G_{k}^{0}(\rho_{k}; \xi) G_{k}^{0}(\rho_{k}; \xi) \right] \]

where identical terms were combined. Finally, reference to (4-23) allows us to do the \( \alpha \) integration in (2-26), giving

\[ \Theta_{q} = \frac{2\lambda}{V} \sum_{k} \left\{ \begin{array}{c}
\frac{n_{k}^{
u} n_{k}^{\nu} B(1+i\xi - p) B(p - p)}{[k^2 + (\rho_{k} - p)^2]^2} \\
- \frac{n_{k}^{
u} n_{k}^{\nu} B(1+i\xi - p) B(p - p)}{[k^2 - (\rho_{k} - p)^2]^2}
\end{array} \right\} \]

The "\( i\eta \)" factor in each of the denominators can be dropped since the various arrangements of theta functions make sure that these denominators cannot vanish. Now, one of the \( \frac{1}{V} \) factors in front of \( \Theta_{q} \) is to go with the \( \phi \) summation while another goes with the \( k \) summation. There remains one volume factor \( \frac{1}{V} \) with no corresponding summation. This makes \( \Theta_{q} \) proportional to \( M_{q} \) and hence \( \Theta_{q} \) vanishes in the limit of infinite volume.

A final important set of diagrams vanish because they violate conservation of momentum. These are well known; see for instance Prange and Klein(14). Diagrams 1-3 (17) and 1-3 (21) are examples of such Feynman graphs.

In the remaining chapters we will have occasion to examine each of the remaining diagrams of figures 1-2 and 1-3.
Notational scheme.

It is convenient to set up a notational convention for later use. We begin with (2-4) and define $\tilde{\alpha}_p$ by the equality $\tilde{\alpha}_p = \frac{1}{\sqrt{\pi}} \tilde{\alpha}_p$. Then the two quantities of interest $\tilde{\alpha} = \sum_p \tilde{\alpha}_p$ and $\tilde{\alpha}_b = \sum_{p \neq p_0} \tilde{\alpha}_p$ become respectively $\tilde{\alpha} = \frac{1}{\sqrt{\pi}} \sum_p \tilde{\alpha}_p$ and $\tilde{\alpha}_b = \frac{1}{\sqrt{\pi}} \sum_{p \neq p_0} \tilde{\alpha}_p$. Taking the limit of infinite volume, introducing a factor of 2 for spin degeneracy, and measuring $\tilde{p}$ in units of $p_F$ (i.e. setting $\tilde{p} = \sqrt{\frac{v}{m}}$), $\tilde{\alpha}$ and $\tilde{\alpha}_b$ can be rewritten as

$$\tilde{\alpha} = \frac{\lambda^2}{(2\pi)^3} \left( \int d^3 \tilde{p} \tilde{\alpha}_{p_F} \right) = \tilde{\alpha}_0 \cdot \frac{2}{4\pi} \int d^3 p \tilde{\alpha}_{p_F},$$

and

$$\tilde{\alpha}_b = \frac{\lambda^2}{(2\pi)^3} \left( \int d^3 \tilde{p} \tilde{\alpha}_{p_F} \right) = \tilde{\alpha}_0 \cdot \frac{2}{4\pi} \int d^3 p \tilde{\alpha}_{p_F}.$$

Clearly $\tilde{\alpha}_{p_F}$ is dimensionless and has the property that if it is equal to $\phi(n\tilde{p})$ it leads to a total annihilation rate of $\tilde{\alpha}_0$ and thus is to be compared with 1. Further, $\tilde{\alpha}_{p_F} \tilde{\alpha}_d$ is such that

$$\int d^3 \tilde{p} \tilde{\alpha}_{p_F} \tilde{\alpha}_d = \tilde{\alpha}.$$ 

Hence define

$$\tilde{\alpha}_{p_F} \tilde{\alpha}_d = \tilde{\alpha} = \tilde{\alpha}_0 \cdot \frac{2}{4\pi} \int d^3 p \tilde{\alpha}_{p_F}.$$

Then $\tilde{\alpha}_{p_F} \tilde{\alpha}_d$ has the units of $\tilde{\alpha}_0$ and is related to $\tilde{\alpha}$ simply by

$$\tilde{\alpha} = \int d^3 p \tilde{\alpha}_{p_F} \tilde{\alpha}_d.$$ 

In numerical calculations from now on we will usually quote $\tilde{\alpha}_{p_F} \tilde{\alpha}_d$ and $\tilde{\alpha}_{p_F} \tilde{\alpha}_d$. 
Chapter 3
KAHANA'S THEORY OF POSITRON ANNIHILATION

Introduction.

Kahana has recently published a theory of the total annihilation rates for metals which agreed quite well with the results of Bell and Jörgensen for the alkalis and aluminium. Since then it has been found that this agreement extends to the rare-earth metals as well\(^{16}\). In this chapter the theory of K-II is sketched with emphasis on the angular correlation problem. We work entirely with the partial annihilation rate \(Q_p\) rather than with the total rate \(\bar{Q}\) as is done in K-II. The lattice is included in the derivation of the effective electron-positron potential. However, the formalism becomes rather cumbersome and so is not carried beyond this point, even though most of the manipulations involved in the rest of the chapter can be done when the lattice is included.

In the high density limit (first order ladder graph), an expression for the partial annihilation rate \(Q^{(1)}_p\) is given which includes both continuum and plasmon contributions. It is found that \(Q^{(1)}_p\) is non-zero for both \(\psi_1 \psi_0\) and \(\psi_1 \psi_2\). This differs from the result given in K-II where the entire contribution to \(Q^{(1)}_p\) from the first order ladder graph, with dynamic effective potential, is interpreted incorrectly to lie in the range \((0, \gamma_f)\). This has no effect on the total annihilation rate but is crucial for the angular correlation problem in the region \(\psi_1 \psi_2\). The variation of \(Q^{(1)}_p\) with \(\gamma_f\) for \(\psi_1 \psi_2\) is investigated in detail, while the case \(\psi_1 \psi_2\) is considered in Chapter 6.

The discussion then turns to the total annihilation rate in the high density limit and its extension to more realistic metal...
densities. The Bethe-Goldstone-type equation needed to do this is not derived in K-II, but for completeness a derivation of this integral equation is given in an appendix and its numerical evaluation is reconsidered. Finally we return to the high density limit. Kahana finds that the total annihilation rate in this limit can be described quite well by replacing the dynamic potential in the first order ladder graph by its static limit provided a correction is made for the plasmon. The question of whether or not the static potential also gives a good description of the angular correlation curve in the region $\varphi < \varphi_c$ is mentioned.

The effective electron-positron potential.

The simplest approximation to the electron-positron correlation function taking into account the electron-positron force is the first order ladder graph shown in figure 3-1. Its contribution to the two-body Green's function is

$$G_{ep}(\mathbf{x}; \mathbf{x'}, \mathbf{y}; \mathbf{y'}) = i \left[ \delta^4(\mathbf{x} - \mathbf{x'}) \delta^4(\mathbf{x'} - \mathbf{y'}) G^e(\mathbf{x}; \mathbf{y}) G^e(\mathbf{x'}; \mathbf{y'}) G^p(\mathbf{x}; \mathbf{y}) G^p(\mathbf{x'}; \mathbf{y'}) \right]. \quad (3-1)$$

![Figure 3-1](image)

First order ladder diagram representing the interaction of an electron-positron pair through the coulomb potential in the Born approximation.

As it stands, formula (3-1) is not a good description of the
actual physical situation since the simple coulomb inverse square law appears as the potential function between the annihilating pair. Clearly, for a high density gas, the effective interaction between the positron and a given electron of the metal cannot be the same as if the interaction took place in free space. Because of the long range of the coulomb force as compared with the inter-electron distance, the force field of the positron must, on the average, overlap that of many electrons in its vicinity. So besides a direct interaction between the positron and the given electron, we must also account for the interaction of the positron with the other electrons forming the surrounding medium. This positron-medium interaction can be described as a polarization of the medium by the positron, the polarization charge acting to screen out and so reduce the effective electron-positron attraction.

In momentum space the coulomb potential \( V(q) \) must be replaced by the effective potential \( u(q, \omega) = V(q) / \varepsilon(q, \omega) \) where \( \varepsilon(q, \omega) \) is called the dielectric constant of the medium, in analogy with classical electromagnetic theory. This dielectric constant accounts for the polarization of the medium and is in general a function of both space and time (or, since we are in momentum space, of momentum \( q \) and frequency \( \omega \)). The time dependence of the dielectric constant is a reflection of the finite inertia of

\*(This is an oversimplification of the true situation in a metal. In writing \( u(q, \omega) \) as a function of \( q \) only, it is implicitly assumed that the effective potential is local, which is not so in a real metal.)*
the surrounding medium which does not permit instantaneous reaction to the positron presence. This response of the system to the positron presence is to a large extent determined by the coulomb repulsions existing between the electrons of the medium. It is well known that it can be partially accounted for by summing the series of diagrams shown in figure 3-2. Each term of figure 3-2 represents a possible interaction of the positron with the given electron. The first is through a direct instantaneous coulomb interaction. The second is through an intermediate excitation of the medium by the positron in the form of a hole-particle pair which can then propagate before final de-excitation on interaction with the given electron. Higher order terms differ from the second order term only in the number of such intermediate excitations and subsequent de-excitations of a hole-particle pair.

Figure 3-2

Diagrams which must be summed in order to get a good description of the effective electron-positron force inside a metal.

The effective electron-positron potential \( u(k, k') \), defined as the sum of all the diagrams of figure 3-2, satisfies the integral equation represented schematically in figure 3-3.
Thus \( u(\mathbf{x}, \mathbf{x}') \) satisfies

\[
  u(\mathbf{x}, \mathbf{x}') = u(\mathbf{x}, \mathbf{x}') - 2i \int \! d^{3} \lambda d^{3} \sigma \sqrt{\left( \mathbf{x} - \mathbf{x}' \right) \cdot \mathbf{G}_e(\mathbf{z};3) \mathbf{G}_e(\mathbf{z};3') u(3,3') .
\]

The factor of 2 in front of the second term on the right hand side enters because of spin degeneracy. Note that a slight modification in the Feynman rules is implied in this equation. Instead of the usual \( u(\mathbf{x}, \mathbf{x}') \), there appears \( u(\mathbf{x}, \mathbf{x}') - \varphi(\mathbf{x}, \mathbf{x}') \mathcal{S}(\mathbf{x}, \mathbf{x}') \). This can be done provided that the integration \( \int d^{3} x d^{3} \sigma' \) which goes with \( u(\mathbf{x}, \mathbf{x}') \) is now changed to \( \int d^{3} x d^{3} \sigma' \).

Because of the invariance of \( u(\mathbf{x}, \mathbf{x}') \) and \( \mathbf{G}_e(\mathbf{x}, \mathbf{x}') \) under translation of the system through a primitive translation vector \( \mathbf{F} \), it is clear from the iterative solution of equation (3-2) that the effective potential must also be invariant under translation of the system through \( \mathbf{F} \). That is,

\[
  u(\mathbf{x} + \mathbf{F}, \mathbf{x}') = u(\mathbf{x}, \mathbf{x}') \quad \text{for all } \mathbf{x}, \mathbf{x}' .
\]

From this relationship it is concluded that \( u(\mathbf{x}, \mathbf{x}') \) can be written in the form

\[
  u(\mathbf{x}, \mathbf{x}') = \frac{1}{\mathbf{\chi}_n} \int_{K_n} \! d\mathbf{q} \mathcal{G}(\mathbf{x}, \mathbf{x}') \mathcal{S}(\mathbf{q}) \mathcal{S}(\mathbf{q} - \mathbf{F}) u(0,0) ,
\]

where \( \mathbf{\chi}_n \) is an inverse lattice vector and \( \mathbf{q} \) is an unrestricted
momentum. In the limit of no crystal potential, the dependence in (3-3) drops out. The effective potential then depends only on the distance between the electron and the positron, and not on their actual position in the metal. However, this is not the case when the crystal field is taken into account. Picture an electron-positron pair inside some primitive cell of the metal. Let \( d \) denote the distance between them; if \( d \) is left unchanged but the pair is moved around in the cell, the force between them will in general change since the position of the pair relative to the fixed ion cores changes. It is clear, though, that the situation must be the same in all primitive cells: i.e. if both particles are translated through \( \gamma \), the potential between them is unchanged.

The effective potential \( u(\kappa; \kappa') \) breaks up quite naturally into two parts: a local part which can be denoted by \( u_1(\kappa; \kappa') \), and a non-local part denoted by \( u_{n.1}(\kappa; \kappa') \). These are given respectively by

\[
u_1(\kappa; \kappa') = \frac{1}{V} \sum_{\kappa_1} \frac{d^2 \kappa}{d^2 \kappa_1} \left[ \int V \omega \left. -i \omega(t-y) \right] \right] \tilde{u}(\kappa_1; \kappa; \omega)
\]

and

\[
u_{n.1}(\kappa; \kappa') = \frac{1}{V} \sum_{\kappa_1} \frac{d^2 \kappa}{d^2 \kappa_1} \left[ \int V \omega \left. -i \omega(t-y) \right] \right] \tilde{u}(\kappa_1; \kappa; \omega).
\]

The non-local part of the potential corresponds to the possibility of umklapp type transitions in which the electron-positron pair could pick up an amount of momentum \( \gamma \), from the translational motion of the lattice. Such processes could clearly lead to contributions to the tails of the angular correlation curve.
It is not our intention here to make an estimate of this effect but we simply note that it is a possible process in real metals which is absent in the case of an electron gas.

If non-local field corrections are neglected, the local part of the effective potential $u_L(x, x')$ still contains traces of the presence of the lattice. In Appendix I an approximate solution of the integral equation (3-2) is obtained for $u_L(x, x')$. It is found that $u_L(x, x') = u_0(x, x') = \frac{\mu^2}{\epsilon(x, x')}$ with

$$
\epsilon(x, x') = 1 + \frac{2i}{V} \sum_{l,l'} \int \frac{d^3k}{(2\pi)^3} \epsilon(k, l') c^*_l(x, k) c^*_{l'}(k, x') c_{l'}(k, x') c_l(x, k),
$$

(3-6)

where $l$ and $l'$ are band indices, and $x$ is a crystal momentum restricted to the first zone. If the specific representation of the Fourier transform of the free electron propagator is introduced in (3-6), there results the dielectric constant given by Ehrenreich and Cohen (n), in the zero temperature limit. (Their derivation of this dielectric constant was based on a density matrix approach in a self consistent field framework.) In a real metal, (3-6) replaces the effective potential given in K-II. In fact, in the limit of no crystal potential, (3-6) becomes

$$
\epsilon(x, x') = 1 + \frac{2i}{V} \sum_{l,l'} \int \frac{d^3k}{(2\pi)^3} \epsilon_l(k, l') c^*_l(x, k) c^*_{l'}(k, x') c_{l'}(k, x') c_l(x, k),
$$

(3-7)

where $x$ is now unrestricted. Expression (3-7) is the well known dielectric constant for an interacting electron gas in the random phase approximation. To carry out a calculation with (3-6) would be a major project requiring a knowledge of the Bloch states for a given metal. For simplicity all formal calculations from this point on will be carried out in the limit of complete translation-
al symmetry, although if this restriction were lifted most of
the manipulations would still remain valid.

Partial annihilation rate in the high density limit.

If the coulomb potential in (3-1) is replaced by the dynamic
effective potential $u(r,\omega)$, Kahana's high density theory is ob-
tained. In this limit the partial annihilation rate $\hat{\gamma}^{(1)}_f$ is

$$
\hat{\gamma}^{(1)}_f = \frac{\hbar c}{V^2} \sum_{k_f} \int \frac{d\omega d\epsilon}{(2\pi)^2} G^+ (k_f^+; t_\omega + \epsilon) G^- (p^-; \epsilon) u(k_f^+; \omega + \epsilon) x G^+ (p^-; \epsilon) G^- (p^-; \epsilon')
$$

(3-8)

where Fourier transforms have been introduced. By a series of
algebraic steps almost identical to those described in K-II,
equation (3-8) can be rewritten as

$$
\hat{\gamma}^{(1)}_f = \frac{2\hbar c}{V^2} \int \frac{d\omega d\epsilon}{(2\pi)^2} \frac{u(k_f^+; \omega)}{\omega^2 - \omega - i \eta} G^+ (p^-; \omega + \epsilon) G^- (p^-; \omega + \epsilon')
$$

(3-9)

The $\epsilon$-integration in (3-9) can be done using formula (4-23).

Thus

$$
\hat{\gamma}^{(1)}_f = \frac{2\hbar c}{V^2} \int \frac{d\omega}{(2\pi)} \frac{u(k_f^+; \omega)}{\omega^2 - \omega - i \eta} \frac{\Theta(p^- - k_f^+ - \epsilon) \Theta(p^- - p) - \Theta(p^- - k_f^+ - \epsilon) \Theta(p^- - p)}{p^- (p^- - k_f^+ - \epsilon - \omega - i \eta)}. 
$$

(3-10)

It is clear from (3-10) that $\hat{\gamma}^{(1)}_f$ is nonzero for $p>\epsilon_f$ as well as
for $p<\epsilon_f$. This was overlooked in K-II. Suppose we worked with
$\hat{\gamma}$ rather than with $\hat{\gamma}^+_f$. There would then be an extra $p$ sum-
mation in equation (3-10) and it would be possible to change the
$p$ variable in the second term of (3-10) to a new variable $q$ by
making the transformation \( f \rightarrow f' \). But this transformation changes \( \Theta(f-p_F) \Theta(p_F-1-f) \) to \( \Theta(f-p_F) \Theta(1+f-p_F) \). Dropping the \( f \) summation now to get \( \Theta_f \) from \( \Theta \) would lead to the incorrect conclusion that \( \Theta_f = 0 \) for \( f > p_F \). This is precisely what was done in K-II; of course this has no effect on the total annihilation rate \( \Theta \), but certainly affects the angular correlation problem. It is therefore necessary to re-examine the variation of \( \Theta_f^{(0)} \) with \( f \) using the correct expression (3-10). In this chapter only the region \( f < p_F \) will be investigated. For \( f < p_F \), equation (3-10) becomes

\[
\Theta_f^{(0)} = \frac{2}{\sqrt{2}} \int_{-\infty}^{+\infty} \frac{u(k,\omega)}{k^2 - \omega^2 - \omega + i\eta} \frac{\Theta(1+f-p_F)}{\rho^2 -(f-k)^2 - \omega + i\eta} \, dk.
\] (3-11)

To do the \( \omega \) integration, the singularities of the effective potential \( u(k,\omega) \) as a function of the complex variable \( \omega \) are needed. These are described in K-II. Summarizing, \( u(k,\omega) \) has a cut extending from \( -(k+2\pi p_F) \) to 0 just above the real axis, and from 0 to \( i(k+2\pi p_F) \) just below. For \( k < k_a \) (the plasmon cut-off) there is an additional pole at \( \omega = 1\Re \) (the plasmon pole). Following Kahana, the \( \omega \) integration in (3-11) could now be done by closing the contour above (or below), leading to a clear split of \( \Theta_f^{(0)} \) into a continuum contribution (from the cut) and a plasmon contribution (from the pole \( \Re \)). We prefer not to do this here. Instead, the integral along the real axis in (3-11) is changed to one along the imaginary \( \omega \) axis and a single expression for \( \Theta_f^{(0)} \) results, including both continuum and plasmon contributions. For the details see Appendix II. There the expression for \( \Theta_f^{(0)} \) is reduced to a double integral and evaluated numerically.
Variation of $\Phi^0_{\rho}$ with momentum. The quantity $\Phi^0_{\rho}$ is dimensionless and has the property that if it were equal to $\Theta(\cdot - \cdot)$ its contribution to the total annihilation rate would be $\Phi^*$ (the Sommerfeld annihilation rate). Also plotted for comparison is $\Phi_{\rho,\nu}^{0*}$ equal to $\Phi_{\rho,\nu}^0$ with the dynamic effective potential replaced by its static limit.

The results are tabulated in the appendix and shown graphically in figure 3-4. The variation of $\Phi^0_{\rho}$ with $\rho$ is quite large. For $\alpha = 0.2$ (i.e. $\alpha = \frac{1}{4}$) the value of $\Phi_{\rho,\nu}^{0*}$ at $\tau = 0.9$ is about 22% larger than its value at $\tau = 1$. Since there are many more passive sea electrons around $\tau = 1$ ($\rho_0$) than around $\rho = \infty$, this 22% variation is important. Suppose that it is neglected and $\Phi_{\rho,\nu}^{0*}$ is
set equal to its value at \( \xi = 0 \) multiplied by \( \Theta (\xi - \eta) \). This leads
to a contribution of 2.06 \( Q^0 \) to the total annihilation rate. If
on the other hand a curve \( \alpha + b \xi + c \xi^2 \) \( (\langle R_{\xi}^0 \rangle \leq 2.055 + 0.451 \xi + 0.141 \xi^2) \)
is fitted to the numerical results of figure 3-4 and the result
is averaged over the electron sea, we get \( \langle R_{\xi}^0 \rangle \equiv \frac{1}{\frac{1}{2}} \langle R_{\xi}^0 \rangle = 2.46 \langle Q^0 \rangle \)
which is considerably larger than 2.06 \( Q^0 \). At this point it
would be possible to evaluate \( Q_{\xi}^n \) for \( \xi > 0 \) (i.e. \( R_{\xi}^0 \)) and to
determine the contribution to the total annihilation rate in the
high density limit by writing \( Q_{\xi}^n = Q_{\xi}^0 + Q_{\xi}^n \) with \( R_{\xi}^0 = \frac{1}{\frac{1}{2}} \langle R_{\xi}^0 \rangle \). Since we know \( \langle R_{\xi}^0 \rangle \) we would need only \( Q_{\xi}^n \). However it is more
convenient to evaluate \( Q_{\xi}^n \) directly from (3-9).

**Total annihilation rate in the high density limit.**

The contribution to the total annihilation rate from (3-9) is

\[
Q_{\xi}^n = \frac{1}{\frac{1}{2}} \langle R_{\xi}^0 \rangle = \frac{2}{\sqrt{\xi}} \sum \int \frac{d \omega i}{\omega} \frac{u(\xi, \omega)}{k^2 \omega - i\eta} Q(\xi, \omega)
\]

with

\[
Q(\xi, \omega) = \frac{1}{\sqrt{\xi}} \sum \int \frac{d \xi}{\omega} \langle \xi \rangle \langle \omega \rangle C^e(\xi, \omega + i\epsilon) C^e(\xi - \xi \epsilon) .
\]

Except for a trivial multiplicative factor, (3-12) is equation
(17) of K-II. Following K-II, completing the contour in (3-12)
above would lead to a clear split of \( Q_{\xi}^n \) into a continuum con-
tribution \( Q_{\xi}^{n, \text{cont}} \) and a plasmon contribution \( Q_{\xi}^{n, \text{plas}} \). The
resulting expressions for \( Q_{\xi}^{n, \text{cont}} \) and \( Q_{\xi}^{n, \text{plas}} \) are rather awkward to
calculate exactly and an approximate method was used in K-II. To
check on these approximations it was felt worth while to again
change the integral along the real axis in (3-12) to one along
the imaginary axis, giving rise to a single expression for \( Q_{\xi}^n \)
which can readily be evaluated on a digital computer. The results
Parameter Variation of the total annihilation rate (in the high density limit) with electron density. Both continuum and plasmon contributions are included.

are shown in figure 3-5. Our curve agrees very well with the results of K-II and justifies the approximations made there.

Extension to realistic metal densities.

For a very high density electron gas (i.e. $\alpha < 1$), it can be expected that treating the screened coulomb force (proportional to $\alpha$) in the Born approximation would give an adequate description of the electron-positron correlation. But for actual metals, $\alpha$ is usually greater than 2 and the Born approximation is not sufficient. This was first recognized by Kahana and led him to consider the integral equation satisfied by the sum of all ladder diagrams:

$$g_{cp}(\xi \xi', \eta \eta') = g_{c}(\xi \eta) g_{p}(\xi', \eta') - i \sum_{\lambda} g_{c}(\eta \lambda) g_{p}(\xi', \delta_{\lambda}) g_{c}(\lambda \lambda) g_{p}(\xi', \gamma_{\lambda}) g_{p}(\xi', \delta_{\lambda}) g_{p}(\eta' \gamma_{\lambda}).$$
To solve this equation the dynamic effective potential must be replaced by some static equivalent. In K-II $\omega(k;\omega)$ is replaced by $\omega(k,\omega)$; this choice was motivated by the fact that it did not change significantly the results for the continuum contribution $Q^0_{\text{cont}}$ in the high density theory. In this limit (3-114) becomes

$$G_{\gamma}(x,y;\gamma) = G_{\gamma}(x,y;\gamma) - i \{ G_{\gamma}(x,y;\gamma) G_{\gamma}(x,y;\gamma) G_{\gamma}(x,y;\gamma) G_{\gamma}(x,y;\gamma) \} .$$ (2.14)

This integral equation together with the formula for its contribution to $Q_\gamma$ can be reduced to a Bethe-Goldstone type amplitude, with $Q_\gamma$ given by $\lambda/\nu$ times the square of this amplitude. For a derivation of this amplitude see Appendix 3, and for its numerical evaluation refer to K-II. The final results have already been presented in Chapter 2 (figure 2-2). Since one expects some core annihilation, a theory which accounts only for the valence electrons (as in K-II) should lead to a curve for the variation of the total annihilation rate $\mathcal{Q}$ with $\nu$, which is slightly lower than the experimental curve. The agreement between theory and experiment is quite good; it is best around $\nu = 4$. As $\nu$ decreases to 2 the theoretical curve goes up a little faster than indicated experimentally, although aluminium still agrees within the limits of experimental error. The more recent work of Rodda and Stewart on scandium, yttrium, and the rare earth metals also seems to indicate less variation of $\mathcal{Q}$ with $\nu$ than that given in K-II. *

*(This experimental work gives only rates relative to that for aluminium which was taken from work by Bell and Jorgensen. It is worth noting that a small reduction of $\mathcal{Q}$ (experimental) for aluminium would be reflected in all these rates.*)
Momentum ($\tau = \omega t$) dependence of $\epsilon(t)$ for $\lambda_2 = \frac{1}{2}$. Our results are compared with those of K-II.

For this reason it was felt worthwhile to redo the numerical work on the integral equation of K-II using a finer grid, at least for the region $\lambda_2 \geq 2$. The numerical results for the variation of the enhancement factor $\epsilon(t)$ with momentum (in units of $\varphi_f$) are presented in Table 3-1, and are compared in figure 3-6 with the results of K-II (table III) for the case $\lambda_2 = \frac{1}{2}$. Our curve starts below that of K-II for $\tau = 0$ but increases more rapidly with momentum. The net result is that if

**Table 3-1**

<table>
<thead>
<tr>
<th>$\varphi_f$</th>
<th>$\tau = 0.1$</th>
<th>$\tau = 0.3$</th>
<th>$\tau = 0.6$</th>
<th>$\tau = 0.9$</th>
<th>$\epsilon_{\text{plas. added on}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>10.61</td>
<td>10.93</td>
<td>12.00</td>
<td>15.07</td>
<td>0.345</td>
</tr>
<tr>
<td>1.89</td>
<td>3.10</td>
<td>3.15</td>
<td>3.34</td>
<td>3.83</td>
<td>0.136</td>
</tr>
</tbody>
</table>

Momentum ($\tau$ in units of $\varphi_f$) dependence of the enhancement factor $\epsilon(t)$ for $\lambda_2 = 0.5$ and $\lambda_2 = 1.89$. The plasmon contribution must be added to these numbers.
is averaged over the electron sea, we obtain a total annihilation rate \( R \) of \( 2.637 \times 10^3 \) sec\(^{-1} \) which agrees with \( R \) as given in K-II to within 1%. This is an adequate check on both our calculations.

For \( \alpha_s = 1.89 \) the enhancement factor can be written as
\[ \varepsilon(v) \cong 3.095 + 0.488 v^2 + 0.511 v^4 + \varepsilon_{\text{plasm}} \]
which leads to a total annihilation rate of \( 6.66 \times 10^3 \) sec\(^{-1} \). This point has been added to the graph of figure 2-2 and fits quite well with the variation of Kahana's curve.

In the next chapters we will look at some refinements of Kahana's theory to see if this variation is indeed correct. This essentially means that we will make an estimate of some of the remaining diagrams in the expansion of the electron-positron correlation function.

**A final note.**

It was pointed out in the previous section that, provided a correction is introduced for the plasmon, the static potential \( \omega(k, \omega) \) gives a good description of the total annihilation rate in the high density limit. Denote by \( Q^{(n,l)}_\pi \) the partial annihilation rate \( \dot{Q}^{(n)}_\pi \) as given by (3-12) with \( \omega(k, \omega) \) replaced by \( \omega(k, \omega) \). Then \( Q^{(n)} = Q^{(n,l)}_\pi + Q^{(l)}_\gamma \) with \( Q^{(n,l)}_\pi = \sum_i Q^{(n,l)}_i \). The question now arises whether or not a similar statement holds true for the angular correlation problem in the region \( p < q \); i.e. is \( Q^{(n,l)}_\pi \) plus a plasmon correlation constant across the sea also a good approximation to \( Q^{(n)}_\pi \)? Since \( Q^{(n)} + Q^{(l)}_\pi = Q^{(n)} \), the answer to this question clearly depends on how large \( Q^{(l)}_\pi \) is as compared with \( Q^{(n)} \). For \( \alpha = 2 \) (\( \alpha_s = 3.79 \)) we have that \( Q^{(l)}_\pi = 2.19 \) and \( Q^{(n)} = 2.16 \) so that \( Q^{(n)}_\pi \) is negative and equal to \(-.27 Q^{(n)} \). Thus
the average over the sea of $\bar{Q}_{\nu}^{\mu_{1}}$ and of $\bar{Q}_{\mu}^{\nu_{1}}$ differ by more than $10\%$ of $Q_{\nu}$ which is not negligible. It is interesting to compare in detail the variation of $Q_{\nu}^{\mu}$ and $Q_{\nu}^{\mu_{1}} - Q_{\nu}^{\mu_{2}}$ across the electron sea.

In figure 3-4, besides $\bar{Q}_{\nu}^{\mu_{1}}$ as a function of momentum $\varphi$ we have also plotted $Q_{\nu}^{\mu_{1}} - Q_{\nu}^{\mu_{2}}$ and (for $\alpha = .2$) $Q_{\nu}^{\mu_{1}} + Q_{\nu}^{\mu_{2}}$. For $\alpha = .2$, $\bar{Q}_{\nu}^{\mu}$ and $Q_{\nu}^{\mu_{1}} + Q_{\nu}^{\mu_{2}}$ agree well around $\varphi = 0$ but as $\varphi$ increases toward 1 the difference between the two curves also increases. In fact, the variation of $Q_{\nu}^{\mu_{1}} + Q_{\nu}^{\mu_{2}}$ between $\varphi = .1$ and $\varphi = .9$ is less than $10\%$ as compared with $22\%$ for $Q_{\nu}^{\mu_{1}} + Q_{\nu}^{\mu_{2}}$.

Since a large number of electrons occupy states around the Fermi surface, this $12\%$ difference in variation across the sea is what causes the deviation of $Q_{\nu}^{\mu_{1}} + Q_{\nu}^{\mu_{2}}$ from $Q_{\nu}^{\mu_{1}}$. However it is not to be taken too seriously since in order of magnitude it is comparable to the corrections expected from self energy effects. In a fully interacting electron gas the states around the Fermi surface are occupied with probability slightly less than 1. This would obviously decrease $Q_{\nu}$ for $\varphi$ near $\varphi_{0}$ ($\nu < \varphi_{0}$). Positron self energies would have a similar effect. In Chapter 5 we will attempt to answer the following question: Are self energy effects large enough to reduce sufficiently the variation of $Q_{\nu}^{\mu_{1}}$ with momentum so as to bring it into agreement with $Q_{\nu}^{\mu_{1}}$?

*(Numerical values for $\bar{Q}_{\nu}^{\mu_{1}}$ can be found in Appendix 2. As a check on this calculation we have evaluated $Q_{\nu}^{\mu_{1}} - \Sigma Q_{\nu}^{\mu_{1}}$. For $\alpha = 2$ ($\alpha = 3.78$), $Q_{\nu}^{\mu_{1}} = 1.911 Q_{\nu}$, while for $\alpha = 1$ ($\alpha = 1.89$) $Q_{\nu}^{\mu_{1}} = 1.065 Q_{\nu}$. Both these values are in reasonable agreement with the values for $Q_{\nu}^{\mu_{1}}$ given in K-II.)*
Chapter 4

EFFECT OF PARTICLE-HOLE INTERACTIONS ON THE ANNIHILATION RATES

Introduction

Kahana's approach to the problem of calculating the correlation function for an electron-positron pair within an electron gas is essentially one of selective summation of diagrams. That is, of the totality of Feynman graphs representing the electron-positron Green's function, only a specific subset is summed, namely the ladder graphs. From the good agreement of Kahana's theory with experiment, there is little doubt that these are by far the most important. Nevertheless, in this chapter we will examine some of the remaining diagrams (in the limit of no lattice), if only to give added theoretical support to Kahana's work.

Diagrams to be included

It was pointed out in Chapter 2 that self energy effects alone cannot change the total annihilation rate $\Gamma$. This does not mean that all diagrams containing self energy parts can be omitted in calculating $\Gamma$. What it does mean, however, is that those graphs containing exclusively self energy processes can be ignored. Hence in first order perturbation theory the only contribution to $\Gamma$ is from the ladder graph. On the other hand, in second order many new processes must be considered besides the ladder diagram. They can conveniently be divided up into two groups. The first (group 1) contains all graphs representing one self energy process and an extra electron-positron interaction. One member of this group is shown in figure 4-la. The two remaining second order graphs shown in 4-lb and 4-lc constitute the second group (group 2); these rep-
resent the possibility of particle-hole interaction and will be dealt with in this chapter. The processes of group 1 must also be looked at but will be left to Chapter 6.

Figure 4-1

![Diagram]

(a) (b) (c)

A typical member of group 1 is (a). Diagrams (b) and (c) constitute group 2.

Possibility of electron hole-positron interactions.

Begin by considering diagram 4-1b. For definiteness assume some specific time ordering for the various external lines. One such time ordering is shown in figure 4-2 and represents a process in which there is an electron hole-positron interaction. More specifically, the thermalized positron interacts with one of the sea electrons, transferring to it enough momentum so as to knock it above the Fermi sea. The excited particles then propagate with the subsequent interaction of the positron with the electron hole left behind by the excited electron. In this

Figure 4-2

A specific time ordering in 4-1b describing an electron hole-positron interaction.
second scattering process the phase space available to the scattered electron hole is limited to the Fermi sea. This is to be compared with the ladder diagram case where the excited electron-positron pair just scatter off each other a second time; the phase now available for final states of the doubly scattered electron consists of all the states above the Fermi sphere.

From phase space considerations alone then, it can be expected that the contribution to $\theta_f$ from electron hole-positron interactions will be smaller than the ladder graph contribution.

Further, these contributions carry opposite signs. An electron-positron interaction is attractive and so increases the electron density at the positron. On the other hand an electron hole-positron correlation is repulsive, thus decreasing the electron density at the positron and hence the total annihilation rate.

But a slight reduction of $\theta_f$, especially in the region of small $\theta_f$, is precisely what is needed to improve the agreement between theory and experiment. It seems worthwhile then to investigate by just how much such an effect can reduce the annihilation rate.

Contribution to $\theta_f$ from electron hole-positron interactions.

The contribution of diagram 4-1b to the electron-positron Green's function is

$$\begin{align*}
G_{Ep}^{0b}(\k_i, \j_i, \j'_{i}) &= (2)^{\frac{1}{2}} \int D_{\k_i}^0 D_{\j_i}^0 D_{\j'_{i}}^0 U(\j_i; \j'_{i}) U(\j_{i}; \j'_{i}) C_{p}^{0}(\k_{i}; \j) C_{p}^{0}(\j_{i}; \j') \\
&= G_{p}^{0}(\j_{i}; \j) G_{E}^{0}(\k_{i}; \j) G_{E}^{0}(\j_{i}; \j').
\end{align*}$$

(4-2)

Note that in (4-1) the coulomb potential $W(\j_{i}; \j')$ has already been
replaced by the static screened coulomb potential \( u(\mathbf{r}_2; \mathbf{r}_3) \). Introducing Fourier transforms for the various quantities on the right hand side of equation (4-1) and performing the indicated space time integrations, as well as summing over the resulting delta functions, gives

\[
\frac{\omega}{V^2} \sum_{\mathbf{k} \in \mathbb{K}} \int \frac{d\omega' d\mathbf{e}_x d\mathbf{e}_y}{(2\pi)^4} u(\mathbf{k}; 0) u(\mathbf{k}'; 0) G_p^i(\mathbf{k}; \mathbf{k}'', \mathbf{e})
\]

(4-2)

\[
G_c(\mathbf{k}'; \mathbf{q} - \mathbf{q}_z; \mathbf{e}) G_p(\mathbf{k}; \mathbf{r}_1) G_c^*(\mathbf{k}'; \mathbf{r}_2) G_c(\mathbf{k}'; \mathbf{r}_3)
\]

Substituting (4-2) into the prescription for the annihilation rate with emission of two quanta of total momentum \( \pi \) yields

\[
\frac{\omega}{V^2} \sum_{\mathbf{k} \in \mathbb{K}} \int \frac{d\omega' d\mathbf{e}_x d\mathbf{e}_y}{(2\pi)^4} u(\mathbf{k}; 0) u(\mathbf{k}'; 0) G_p^i(\mathbf{k} + \mathbf{q}; \mathbf{e}_x, \mathbf{e}_y) G_c(\mathbf{k}'; \mathbf{e}_z - \mathbf{e}_z + \omega)
\]

(4-3)

\[
G_p(\mathbf{k}; \mathbf{e}_x) G_c(\mathbf{k} + \mathbf{q} - \mathbf{q}_z; \omega) G_c^0(\mathbf{k} - \mathbf{q}_z; \mathbf{e}_z) G_c(\mathbf{k}'; \mathbf{e}_z - \mathbf{e}_z + \omega)
\]

where the \( \mathbf{k} \) and \( \mathbf{q} \) integrations have been performed, giving a delta function \( \delta_{\mathbf{k}', \mathbf{k} + \mathbf{q} - \mathbf{q}_z} \) times a volume element. This delta function has then been used to carry out the \( \mathbf{k}' \) summation. A change of variable from \( \omega \) to \( \nu \), where \( \omega = \epsilon - \epsilon + \omega \), puts (4-3) in the more symmetric form

\[
\frac{\omega}{V^2} \sum_{\mathbf{k} \in \mathbb{K}} \int \frac{d\omega' d\mathbf{e}_x d\mathbf{e}_y}{(2\pi)^4} u(\mathbf{k}; 0) u(\mathbf{k}'; 0) \int \frac{d\mathbf{e}_x}{2\pi} G_p^i(\mathbf{k} + \mathbf{q}; \mathbf{e}) G_c(\mathbf{k}'; \mathbf{e}_z - \mathbf{e}_z + \omega)
\]

(4-4)

\[
\int \frac{d\mathbf{e}_x}{2\pi} G_p(\mathbf{k}; \mathbf{r}_1) G_c^0(\mathbf{k} - \mathbf{q}_z; \mathbf{e}_x, \mathbf{e}_y) \int \frac{d\mathbf{e}_y}{2\pi} G_c(\mathbf{k}'; \mathbf{e}_z - \mathbf{e}_z + \omega)
\]

or
Referring to (4-6), the \( \sigma \)-integration in expression (4-5) can now be done. Eight terms have to be considered. However, only six of these remain after the \( \sigma \)-integration since, for two terms, the integrand has all its poles in the same half plane.

The six remaining terms all contain at least one positron theta function of the form \( \Theta(-\xi) \) which can be used to do the \( k \)-summation. Hence

\[
\Theta^{(\text{bb})}_\xi = \lambda \frac{\alpha}{\pi^2} \sum_{b'} \left[ u(b',0) u(b',0) I(k+q; \xi q' - k' q') \right] \times \left( \frac{\sigma_q}{\pi^2} \right) G_\xi^0 (\xi; z) G_\xi^0 (\xi; \xi + i \eta) \tag{4-5}
\]

where by definition

\[
I(q; q', \eta) = \int \frac{d \xi}{2 \pi} G_\xi^0 (\xi; \xi) G_\xi^0 (\xi; \xi + i \eta) \tag{4-6}
\]

\[
\left[ \frac{\Theta(-\xi) \Theta(-\xi - \eta)}{\xi^2 - \xi^2 - \eta + i \eta} - \frac{\Theta(-\xi) \Theta(-\xi - \eta)}{\xi^2 - \eta + i \eta} \right].
\]

Referring to (4-6), the \( \sigma \)-integration in expression (4-5) can now be done. Eight terms have to be considered. However, only six of these remain after the \( \sigma \)-integration since, for two terms, the integrand has all its poles in the same half plane.

The six remaining terms all contain at least one positron theta function of the form \( \Theta(-\xi) \) which can be used to do the \( k \)-summation. Hence

\[
\Theta^{(\text{bb})}_\xi = \lambda \frac{\alpha}{\pi^2} \sum_{b'} \left[ u(b',0) u(b',0) \right] \begin{align*}
&\frac{\Theta(-\xi) \Theta(-\xi - \eta)}{\xi^2 - \xi^2 - \eta + i \eta} - \frac{\Theta(-\xi) \Theta(-\xi - \eta)}{\xi^2 - \eta + i \eta} \\
&= \frac{\Theta(-\xi) \Theta(-\xi - \eta)}{\xi^2 - \xi^2 - \eta + i \eta} - \frac{\Theta(-\xi) \Theta(-\xi - \eta)}{\xi^2 - \eta + i \eta} \tag{4-7}
\end{align*}
\]
where identical terms have been combined. Note that all the \( i \gamma \) factors are now irrelevant since the various arrangements of theta functions ensure that no denominator has a zero. As expected, \( \hat{\Theta}^{(4)}_T \) is negative. Also note that in the second and fourth terms of (4-7) there still remains a theta function of the form \( \Theta(-1) \) which can be used to carry out another of the summations. But this leads to terms having an extra factor \( 1/\nu \) in front, without a corresponding summation. In the limit of infinite volume these terms vanish. This is clearly a reflection of the fact that there is no positron sea, i.e. these terms are proportional to the positron density which is zero. Hence \( \hat{\Theta}^{(4)}_T \) reduces to

\[
\hat{\Theta}^{(4)}_T = \frac{\lambda}{\sqrt{3}} \sum_{\nu, \lambda} \langle \nu, \lambda | \nu, \lambda \rangle \left[ \frac{\Theta(\xi^2) \Theta(\xi^2 + 1) \Theta(\xi + \xi^2) \Theta(\xi + \xi^2 + 1)}{[\xi^2 - (\xi + \xi^2)^2 - (\xi + \xi^2)^2] \left[ (\xi^2)^2 - (\xi + \xi^2)^2 \right]} \right] .
\]

The first term in (4-8) contributes only if \( f \neq f \), while the second term contributes for all \( f \)'s. To understand this, it is useful to construct momentum space diagrams for the two terms of (4-8) in which the annihilation process is specifically represented.

**Diagrams explicitly indicating the annihilation process.**

First go back to the general expression for \( \Theta_T \) which by
definition is

\[ Q_f = \frac{\lambda}{\sqrt{2}} \int \frac{d^3 \mathbf{k}}{\sqrt{2 \pi}} \int \frac{d^3 \mathbf{\eta}}{\sqrt{2 \pi}} \cdot \psi^{\dagger}(\mathbf{k}) \phi(\mathbf{\eta}) \psi(\mathbf{k}) \psi^{\dagger}(\mathbf{\eta}) \psi(\mathbf{k}) \psi^{\dagger}(\mathbf{k}) |W_1\rangle |W_2\rangle. \] (4-9)

Introduce into (4-9) the Fourier decomposition (1-5) of the field operators. The integrations over \( d^3 \mathbf{k} \) and \( d^3 \mathbf{\eta} \) can then be done and the resulting delta functions used to perform two momentum summations, giving

\[ \mathcal{R}_f = \frac{\lambda}{\sqrt{2}} \sum_{k} \langle W_1 | a_{k}^{\dagger} | W_2 \rangle \langle W_1 | b_{k}^{\dagger} | W_2 \rangle \langle W_1 | a_{-k}^{\dagger} | W_2 \rangle | W_1\rangle |W_2\rangle. \] (4-10)

Now recall that \( \mathcal{R}_f \) (the partial annihilation rate) is equal to the probability per unit time that a system of \( N \) electrons and a single positron in a state \( |W_1\rangle \) will spontaneously make a transition to some arbitrary final state \( |W_2\rangle \) of \( N-1 \) electrons with the emission of a gamma-ray pair of total momentum \( \mathbf{q} \). In other words, it is the square of the amplitude

\[ \langle W_{-1} | \sum_{k} \delta_{k}^{(q)} a_{q-k}^{(q)} | W_1 \rangle \]

for the electromagnetic transition

\[ N_e + 1_p \rightarrow (N-1)e + \frac{2W}{\gamma} \]

in a state \( |W_1\rangle \) in a specific state \( |W_{-1}\rangle \) in an arbitrary state of total momentum \( \mathbf{q} \)

summed over all possible final states \( |W_{-1}\rangle \) :

\[ \mathcal{R}_f = \frac{\lambda}{\sqrt{2}} \sum_{k} \langle W_{-1} | \sum_{k} \delta_{k}^{(q)} a_{q-k}^{(q)} | W_1 \rangle^2. \] (4-11)

It is clear from (4-11) that a knowledge of the final state of the system after the annihilation process has occurred is only indirectly contained in the expression (4-10). Nevertheless,
when the various contributions to $\Theta_{\rho}$ are broken up into individual processes (in the sense of time independent perturbation theory), it is possible to read any desired final state from a suitably constructed graphical representation of ($4$-10). The diagrams required are quite easily derived from the Feynman graphs for the electron-positron correlation function $G_{ep}(\rho, \rho')$. Note that these Feynman graphs represent $G_{ep}(\alpha, \alpha'; \rho, \rho')$ for arbitrary arguments $(\alpha, \alpha'; \rho, \rho')$. To derive $\Theta_{\rho}$ from $G_{ep}(\alpha, \alpha'; \rho, \rho')$, a contraction $\alpha - \alpha' = \alpha_1$, $\rho - \rho' = \hat{\rho}$ is necessary. Diagramatically, this contraction can be represented by joining the free electron end $\alpha_1 (\rho_1)$ with the free positron end $\alpha' (\rho')$ at the space time point $\alpha_1 (\hat{\rho})$. Next a Fourier transformation of the $\hat{\rho}$ and $\hat{\rho}$ dependence of the contracted two-particle propagator must be made and only their $\rho$'th component retained. To within some trivial multiplicative factors, this then gives $\Theta_{\rho}$. In diagram language, the Fourier transformation leads to the association of momenta with the various propagator lines, with conservation of momentum and particles applied at each interaction vertex. At the points $(\alpha_1)$ and $(\hat{\rho})$, the conservation laws do not apply. Instead, at $(\alpha_1)$ two particles, an electron and a positron, are taken out of (inserted into) the system with a corresponding loss (gain) of momentum $\rho$. Now clearly, if at $\alpha$ (time $t$) an electron of momentum $\rho$ and a positron of momentum $\rho'$ are annihilated, they must have been in the system before, i.e. in the wave function $\psi_1$. Hence all processes occurring below the annihilation time $t$ are to be associated with the wave function $\psi_1$. That is, they are interpreted as induced on the non-interacting ground state by the coulomb interactions which change $\psi_1$ into $\psi_1'$, the fully interacting ground state. All processes above time $t$ are similarly
associated with coulomb interaction processes in the conjugate state $\langle \psi_1 \rangle$.

**A first example.**

In order to clarify the above discussion, the following specific example is given. Consider the special time ordering of graph 4-1b shown in figure 4-2. Since all arrow directions are fixed, we are left with no alternative but to consider the annihilation time $t$ as later than both of the interaction times $t_1$ and $t_2$. After Fourier transformation, the corresponding diagram for $Q_4$ is shown in figure 4-3. It can be described as follows.

**Figure 4-3**

A specific time ordering in diagram 4-1b. The double solid horizontal line represents the time at which the annihilation occurs.

follows. At time $t$, an interaction with momentum transfer $\frac{\epsilon}{2}$ occurs between the zero momentum positron and one of the sea electrons. The electron hole and positron hole, and the excited electron and positron, then propagate freely until time $t_2$. At time $t_2$ the excited positron scatters off the electron hole with a transfer of momentum $\frac{\epsilon}{2}$. From time $t_2$ to $t$ we again have free propagation. At $t$ the "annihilation operator" acts, absorbing the excited electron of momentum $\frac{\epsilon}{2}$ and the excited positron of momentum $\frac{\epsilon}{2}$, and filling the electron hole $\frac{\epsilon}{2}$ and the positron hole $\frac{\epsilon}{2}$. The approximation to $\langle \psi_1 \rangle$ (the fully
interacting ground state) used in this term is $|\psi_1\rangle$ (the free ground state) modified by the two coulomb interactions at $t_1$ and $t_2$, while the approximation to the conjugate state $|\psi_1\rangle$ is simply $|\psi_1\rangle$. Further, the final state $|\psi_2\rangle$ of the system is the free ground state with the positron and an electron of momentum $q$ removed. For a contribution it is clear that $q$ must be smaller than $p_F$. This handles the first term of equation (4-8).

A second example.

The diagram representing the second term of equation (4-8) is drawn in figure 4-4. It differs from the first in that now the arrangement of arrows in the free lines forces us to choose the annihilation time between the two interaction times $t_1$ and $t_2$. This diagram can be described in the following way. At time $t_1$, a coulomb interaction between the zero momentum positron and one of the sea electrons occurs, knocking both out of the Fermi sea. The two holes, and the excited particles, then propagate freely until

![Figure 4-4](image)

A second time ordering of 4-1b. The annihilation process occurring at time $t$ is explicitly represented.

annihilation time $t$. At time $t$ the excited positron (of momentum $t$) is absorbed as well as the unexcited sea electron (of momentum $t+\frac{q}{t}$). Also, the electron hole ($t'\frac{q}{t}$) is filled and a positron ($\frac{q}{t}$) is reintroduced. From time $t$ to $t_2$ there is
free propagation of the excited electron \((\xi + \xi' - \xi')\), positron hole
\((\xi)\), newly created positron \((\xi')\), and electron hole \((\xi + \xi)\). At
time \(t\), the excited electron and positron interact to fill res‐
pectively the electron and positron hole. The approximation
used to \(\tilde{W}_1\) is \(\tilde{W}_1\), modified by the coulomb interaction at \(t\),
and that to the conjugate state is \(\tilde{W}_1\) modified by the coulomb
vertices at \(t\). The final state of the system \(\tilde{W}_1\), is \(\tilde{W}_1\) with
electron holes \((\xi - \xi')\) and \((\xi + \xi)\), an excited electron \((\xi + \xi' - \xi')\),
and the positron removed. Clearly there is no restriction of \(\rho\)
in order that there be a contribution from this diagram. This
completes our discussion of diagrams in which the annihilation
process is explicitly represented.

Quantitative estimate of \(\tilde{\Omega}_{\xi}^{(b)}\) for \(\rho = 0\).

The simplest quantitative estimate of (4-8) that one can
make is to specialize to the case \(\rho = 0\). In this limit the
partial annihilation rate \(\tilde{\Omega}_{\xi}^{(b)}\) becomes

\[
\tilde{\Omega}_{\xi}^{(b)}(\rho = 0) = \frac{\lambda}{V} \sum_{\xi', \xi} \langle \xi, \xi' \mid \xi, \xi' \rangle \left[ \frac{\frac{2}{\theta(-q', 1)} \theta(-q'' - q', 1) - \theta(-q, 1)}{[\frac{2}{\theta(-q, 1)} - \theta(-q', 1)] \left[ \frac{2}{\theta(-q, 1)} \theta(-q', 1) \theta(-q, 1) \right]} \right].
\]

(4-12)

In (4-12) change all summations to integrations, measure all mom‐
enta in units of the Fermi momentum \(p_F\) and introduce the parameter
\(\alpha = 1/(\gamma_0 p_F^2) = 1/(1|\xi| p_F^2)\). The resulting expression can be written
as

\[
\tilde{\Omega}_{\xi}^{(b)}(\rho = 0) = \frac{\lambda}{V} \tilde{\Omega}_{\xi}^{(b)}(\rho = 0) \equiv \frac{\lambda}{V} (I_1 + I_2).
\]

(4-12)
with

\[ I_1 = -\alpha^2 \int_0^{\frac{1}{\beta}} \frac{\alpha^2 \beta^2}{\beta^2 + \alpha^2} \frac{1}{(\beta^2 + \alpha^2)^2} \, d\beta \]  

(4-14)

and

\[ I_2 = -\alpha^2 \int_0^{\frac{1}{\beta}} \frac{\alpha^2 \beta^2}{\beta^2 + \alpha^2} \frac{1}{(\beta^2 + \alpha^2)^2} \, d\beta \]  

(4-15)

In integrals (4-14) and (4-15) the potential function \( V(\beta) \) stands for

\[ V(\beta) = \frac{1}{(\beta^2 + \alpha^2 \beta^2 + \alpha^2 \beta^2)^2} \]  

(4-16)

The quantities \( I_1 \) and \( I_2 \) are further reduced and evaluated numerically in Appendix 4. The values of \( \alpha \) used for the calculation were \( \alpha = 1 \), \( \alpha = 0.5 \), and \( \alpha = 2 \), corresponding roughly to the range 2 to 4 for the parameter \( a_0 \). The results are tabulated in Table A4-I. The sum of \( I_1 \) and \( I_2 \) is \( \alpha_{HF}^{(0)} \), a dimensionless number. It has the property that if \( \alpha_{HF}^{(0)} = 1 \) for \( \beta = 1 \) and is zero otherwise, then the total annihilation rate derived from \( \alpha_{HF}^{(0)} \) is the Sommerfeld rate \( \alpha^0 \). In this sense \( \alpha_{HF}^{(0)} \) is to be compared with \( \alpha \). In figure 4-5 \( \alpha_{HF}^{(0)} \) is plotted as a function of \( \alpha \). For \( \alpha = 1 \), the electron hole-positron interaction reduces the annihilation rate by approximately 6% of \( \alpha^0 \), while for \( \alpha = 2 \) the reduction is 10% of \( \alpha^0 \). This reduction is appreciable, but it will be shown in the next section that it is not real in the sense that electron hole-electron interactions almost completely cancel out this reduction.
Effect of electron hole-positron interaction on the annihilation rate.

If the variation with \( \rho \) of the partial annihilation rate \( Q_F^{\rho} \) is neglected, then its contribution to the total rate is \( \bar{Q} \cdot Q_F^{\rho} \).

Possibility of electron hole-electron interactions.

We now turn our attention to diagram \( \gamma - lc \). For fixed reference it is again convenient to impose a specific time ordering on the four external lines of \( \gamma - lc \). One such time ordering is shown in figure \( \gamma - 6 \), and we compare this with the diagram of figure \( \gamma - 2 \). At time \( t_1 \) an interaction between the zero momentum positron and a sea electron occurs. In the interval \( t_1 \) to \( t_2 \), there is free propagation of the excited pair and their corresponding holes. At time \( t_2 \) a second interaction takes place. The correlation now is between the excited electron and the electron hole, while in \( \gamma - 2 \) it is the excited positron and the electron hole which are involved.

A possible time ordering of \( \gamma - lc \) describing an electron hole-electron interaction.
The phase space available as final states in this second scattering process are the states below the Fermi sphere in the case of the electron hole, and those above in the case of the excited electron. Note that these phase space restrictions are slightly more severe than in the case of the electron hole-positron interaction; there, no phase space restrictions occur on the positron final states. Hence it can be expected that the contribution to the annihilation rate from the electron hole-electron interaction will be smaller in magnitude than that from the electron hole-positron interaction. Further, these two contributions are of opposite sign since an electron hole-electron correlation is attractive and must lead to a positive contribution to $\mathcal{A}$.

**Contribution to $\mathcal{A}$ from electron hole-electron interactions.**

The contribution to the two-body correlation function coming from diagram 4-1c is:

$$G_{ep}^{(4c)}(\mathbf{k}_{\pi}; \mathbf{q}'; \mathbf{p}) = - (i)^3 \int d\mathbf{p}_1 d\mathbf{p}_2 d\mathbf{p}_3' d\mathbf{p}_4' \ u(\mathbf{p}_1, \mathbf{p}_2) u(\mathbf{p}_3, \mathbf{p}_4') \ G_{\pi}^{(3)}(\mathbf{k}_{\pi}) G_{e}^{(3)}(\mathbf{p}_1, \mathbf{p}_2) \ G_{e}^{(3)}(\mathbf{p}_3, \mathbf{p}_4').$$

(4-16)

Fourier transforming (4-16), it becomes

$$G_{ep}^{(4c)}(\mathbf{k}_{\pi}; \mathbf{q}'; \mathbf{p}) = \frac{i}{4} \int \frac{d\omega d\mathbf{q} d\mathbf{q}' d\mathbf{p}}{(2\pi)^4} \ u(\mathbf{q}, \mathbf{q}') u(\mathbf{q}', \mathbf{q}) \ G_{\pi}^{(3)}(\mathbf{k}_{\pi} - \mathbf{q}) \ G_{e}^{(3)}(\mathbf{k}_{e} - \mathbf{q}') \ G_{e}^{(3)}(\mathbf{p} - \mathbf{q}).$$

(4-17)

The momentum space diagram representing (4-17) is shown in figure 4-7g. This last expression simplifies somewhat if the variable $\mathbf{q}'$
is changed to $\alpha$ by the linear transformation $\alpha' = \omega' \cdot \alpha$. Equation (4-17) can then be rewritten as

$$G^{(c)}(\alpha x'; \gamma^+ \gamma) = \frac{4 \pi}{V} \int_{\mathbb{R}^3} \frac{d^3k}{(2\pi)^3} \frac{i}{(k+\gamma) \cdot (k-\gamma)} \int \frac{d\omega}{2\pi} \frac{G^0_e(k; \omega)}{G^0_e(k'; \omega + \omega')}$$

$$\times \int \frac{d\omega'}{2\pi} \frac{G^0_e(k'; \omega')}{G^0_e(k-\gamma'; \omega') \omega' + \omega') \int \frac{d\omega}{2\pi} \frac{G^0_e(k'; \omega)}{G^0_e(k+\gamma'; \omega)}}$$

(4-18)

Insert (4-18) into the general expression for the partial annihilation rate $G^c_\gamma$ and do the $d^3k$ and $d^3x$ integrations. A volume factor and a delta function $\delta_{\gamma, \infty}$ result. The $k$ summation can then be carried out, giving

$$G^{(c)}_{\gamma} = \frac{\lambda (\gamma^2)^2}{V} \int \frac{d^3k}{(2\pi)^3} \frac{u(k; \omega) u(k'; \omega')}{G^0_e(k; \omega) G^0_e(k'; \omega + \omega')}$$

(4-19)

$$\times \int \frac{d\omega}{2\pi} \frac{G^0_e(k'; \omega')}{G^0_e(k-\gamma'; \omega') \omega' + \omega') \int \frac{d\omega}{2\pi} \frac{G^0_e(k'; \omega)}{G^0_e(k+\gamma'; \omega)}}$$

But

$$\int \frac{d\omega}{2\pi} \frac{G^0_e(q-\gamma; \omega) G^0_e(q-\gamma'; \omega)}{(q-\gamma)^2 - m^2 + i\epsilon} = \frac{\theta(\gamma - m) \theta(-q + m) - \theta(q - m) \theta(-q + m)}{(q-\gamma)^2 - m^2 + i\epsilon)}$$

(4-20)

If equation (4-20) is used in (4-19), the $k$ summation can be done by making use of the positron theta function of the form $\theta(-\omega)$. Two terms arise:
The two terms in (4-21) are actually identical. To transform the second term into the first, make the following transformations in order: \( \eta \rightarrow -\frac{t}{\nu} \), \( \alpha \rightarrow -\omega \), and then change \( \omega (\nu) \) to \( \omega (\nu') \) by setting \( \omega = \omega - \alpha \) \( (\omega = \omega - \alpha') \). This yields

\[
\begin{align*}
\Theta^{(\alpha)}_\eta &= \frac{\lambda \nu^2}{\nu^2} \sum_{n=\pm} u(q',0) u(q,0) \int \frac{d\omega}{2\pi} \frac{2i\Theta(\nu)}{\nu^2 + i\nu + i\eta} \int \frac{d\omega'}{2\pi} G^0_\nu (q+q';\omega) G^0_\nu (q';\omega + \omega') \\
&+ \int \frac{d\omega}{2\pi} G^0_\nu (q;\omega) G^0_\nu (q;\omega + \omega') \int \frac{d\omega'}{2\pi} G^0_\nu (q+q';\omega') G^0_\nu (q';\omega') \frac{i\Theta(\nu)}{\nu^2 + i\nu + i\eta}.
\end{align*}
\]  

(4-22)

It is easy to verify that

\[
\int \frac{d\omega}{2\pi} G^0_\nu (q+q';\omega) G^0_\nu (q';\omega + \omega') = C \left[ \frac{\Theta(q+q'-\nu) \Theta(p-q')}{x^2 - (q+q')^2 + i\eta} - \frac{\Theta(q+q'+\nu) \Theta(p+\nu)}{x^2 - (q+q')^2 - i\eta} \right].
\]  

(4-23)

Using (4-23) the \( \alpha \) integration in (4-22) can be done by contour integration in the complex \( \omega \)-plane. This gives three terms:

\[
\Theta^{(\alpha)}_\eta = \frac{\lambda \nu^2}{\nu^2} \sum_{n=\pm} u(q',0) u(q,0) 2i \Theta(\nu) \nu^2 \left[ \\
- \frac{i \Theta(q+q'-\nu) \Theta(p-q')}{(q+q')^2 - i\eta} \right] \frac{\Theta(q+q'+\nu) \Theta(p+\nu)}{(q+q')^2 + i\eta}
\]

(4-24)
All the "(\eta)" factors in (4-24) can be dropped. The theta functions in the numerator of each term properly restrict the range of the variables $\eta$ and $\eta'$ so as to keep the denominators from having a zero. The first two terms are non-zero only if $p' > p_F$, while the third vanishes unless $p > p_F$. These three terms are of the type which would occur in time independent perturbation theory and momentum space diagrams explicitly exhibiting the annihilation process for each are given in figure 4-7. Also shown are three other graphs which would have entered had we not put together the two terms of (4-21) in going to (4-22). Similar diagrams have already been discussed in detail in this chapter, so we will not describe these further.

Quantitative estimate of $R_\eta^{(c)}$ for $\eta = 0$.

To get an idea of the magnitude of (4-26) again take the simple case $\eta = 0$. In this limit (4-26) becomes

\[
R_\eta^{(c)} = \frac{2\lambda}{\sqrt{2}} \sum_{\eta', \eta''} U(\hat{\eta}, \hat{\eta}') U(\hat{\eta}', \hat{\eta}'') \left[ \frac{\delta(\eta_{\eta''} - \eta_{\eta'}) \delta(\eta'_{\eta''} + \eta_{\eta'}) \delta(\eta'_{\eta'} - \eta_{\eta''})}{[-\eta_{\eta'}^2][\eta_{\eta'}^2 - (\eta'_{\eta'} + \eta_{\eta''})^2]} \right]
\]

(4-25)

where only two terms appear since for $\eta = 0$ the last term in (4-24) is zero. If in (4-25) all summations are changed to integrations, all momenta measured in units of $p_F$, and the parameter $\alpha$ is introduced, the resulting expression can be written as
Diagram (g) represents the Fourier transform of 4-lc. When all possible time orderings in (g) are taken, six graphs arise. These are shown in (a) to (f). The double solid horizontal lines represent the time at which the annihilation is to be considered as taking place.
with

\[ \phi_1 = \alpha^2 \int \frac{d^3 q}{(2\pi)^3} \frac{1}{q^2 + m^2} \int \frac{d^3 \bar{q}}{(2\pi)^3} \frac{1}{\bar{q}^2 + m^2} \]  

and

\[ \phi_2 = \alpha^2 \int \frac{d^3 q}{(2\pi)^3} \frac{1}{q^2 + m^2} \int \frac{d^3 \bar{q}}{(2\pi)^3} \frac{1}{\bar{q}^2 + m^2} \]  

All the angular integrations in (4-27) and (4-28) can be done analytically and the resulting twofold integrals evaluated numerically. For details see Appendix 4. In Table A\textsuperscript{4-2} of this appendix, numerical values for \( \phi_1 \) and \( \phi_2 \) are given for three values of \( \alpha \). The sum of \( \phi_1 \) and \( \phi_2 \) giving \( \phi_{\text{inc}}^{(4c)} \) is plotted in figure 4-8. This cancels against the contribution to \( \phi_{\text{int}}^{(4c)} \) from the electron hole - positron interaction (figure 4-5). The sum of these two effects still amounts to a reduction of the annihilation rate. However, this reduction is rather small (about 2\% of \( \phi^* \)).

**Figure 4-8**

Effect of electron hole-electron interaction on the annihilation rate.
there being almost no variation with the valence electron density. For the total annihilation rate it would appear then that the distortion introduced into the system by the positron force is well described by the ladder graphs, with further refinements altering Kahana's theoretical results by no more than a few percent of $Q^*$. 

In conclusion, it must be stressed that in our investigation of particle-hole correlations no enhancement effects have been accounted for. Once the electron-positron pair is excited, we have considered the possibility of either a positron or an electron correlation with the charge disturbance left behind in the passive electron sea. But then the excited pair annihilates without any direct interaction between them. To account for such a direct interaction, higher order diagrams consisting of a particle-hole interaction and a further series of ladder processes would have to be included. Two examples of the diagrams we have in mind are shown in figure 4-9, for the case of a positron-electron hole correlation. From the work of Kahana, it can be expected that these enhancement effects are very important. But in view of the

Figure 4-9

Higher order diagrams accounting for enhancement effects.
cancellation found between electron hole -positron and -electron interactions, it is not worth while to pursue the calculation further since this cancellation must remain to all orders. For instance, with each of the diagrams (a) and (b) of figure 1-9 one can associate another in which the electron hole -positron interaction part is replaced by an electron hole -electron interaction part, and these cancel against (a) and (b). This type of cancellation will be discussed in detail in Chapter 6. It is worth mentioning here the work of a Japanese group (14) who have discussed the electron hole -positron interaction with enhancement effects included. Their work is based on a Bohm-Pines theory for determining the effective screened coulomb force. They obtain a correlation function for the electron-positron pair within a metal by solving a generalized Bethe-Goldstone equation which embodies the positron-electron hole interaction as well as the positron-electron interaction. Their conclusion is that the annihilation rates found in K-I are appreciably reduced. This is of course as expected but it is not a complete picture. The reduction is an overestimate because of the omission of the electron hole-electron interactions and because of the use of the Bohm-Pines potential.

As mentioned at the outset of this chapter, there are other second order diagrams which can change the total annihilation rates. These are the diagrams of group 1 which consists of all second order graphs describing a self energy process, and an extra electron-positron interaction connecting the electron part of the graph to the positron part. Since each of the diagrams of group 1 contains a self energy part, it is natural to first examine the effect of pure self energy processes on the angular correlation
of the annihilation gamma-rays. These processes in the region \( p < q \) will be the subject of Chapter 5, while the region \( p > q \) is left to the first part of Chapter 6. There we will also consider the contribution to \( Q_p \) (for \( p > q \)) from the second term of \((4-9)\) and the last term of \((4-24)\). It is not until the second part of Chapter 6 that we return to the diagrams of group 1.
Chapter 5.
EFFECT OF SELF ENERGIES ON THE ANGULAR CORRELATION CURVE FOR MOMENTA SMALLER THAN THE FERMI MOMENTUM

Introduction.

The variation of the partial annihilation rate $\Gamma_1$ with momentum across the Fermi sea is of great interest. It was found in Chapter 3 that the first order ladder graph with full dynamic effective potential gave a much greater variation of $\Gamma_1$ across the electron sea than when the dynamic potential is approximated by its static limit. However, it was pointed out that this variation would be reduced somewhat if self energy effects were included. In this chapter we investigate this problem in the high density limit and come up with the following rather remarkable conclusion. When we include in $\Gamma_1$ the three first order graphs shown in figure 5-1 (namely the first order ladder, electron self energy, and positron self energy diagrams) we obtain a variation of $\Gamma_1$ with momentum almost identical to the variation of $\Gamma_2^s$, where $\Gamma_2^s$ is given by the first order ladder graph with the dynamic potential replaced by its static limit. Further, if the result in the static limit is corrected for the plasmon by adding a constant factor (across the sea) as given in K-II, then to within a few percent the agreement is extended to magnitudes as well. Thus, for $\rho - \rho$, replacing the dynamic potential in the first order ladder graph by its static limit has essentially the same effect as including self energy diagrams, provided of course a correction is made for the plasmon. This conclusion should give us confidence that the enhancement factor $\mu(Q)$ as given in K-II
Figure 5-1

(a) (b) (c)

First order ladder (a), electron self energy (b), and positron self energy (c) diagrams.

is quite adequate even near the Fermi surface.

Electron self energies.

For a fully interacting electron gas, the probability of occupation of a state of momentum $p$ ($Q(p)$) is not a simple theta function $\Theta(p-P_F)$: 1 inside the Fermi sphere and zero outside. There is now a finite probability of finding an occupied state outside the Fermi sphere or of finding a vacant state inside. That is, $Q(p)$ is slightly less than 1 for $p = P_F$, with the deviation from 1 increasing as $p$ increases towards $P_F$. As we cross the Fermi sphere there still remains a discontinuous jump in $Q(p)$ but it does not fall all the way to zero. In fact, $Q(p)$ remains appreciable up to a distance of the order $P_F$ away from the Fermi surface. Figure 5-2 shows $Q(p)$ up to first order in perturbation theory for the parameter $\alpha_z = 2$ which corresponds roughly to sodium. The general features of the electron probability of occupation function shown in this figure are not destroyed in higher order perturbation theory. For instance, Luttinger \(^{(11)}\) has shown that the discontinuity at $P_F$ is a general property of normal Fermion systems and remains to all order of the perturbation series. It is precisely this discontinuity which is used to define the Fermi surface.
Figure 5-2

\[ Q(x) \]

\[ \text{Momentum } (x) \text{ in units of } \varphi_f \]

\[ Q(x) \text{ gives the probability of occupation of a state of momentum } x \text{ by an electron in first order perturbation theory.} \]

in the case of an electron gas (Migdal\(^{(n)}\)).

It is clear from figure 5-2 that taking into account the true momentum distribution \( Q(x) \) in an interacting electron gas leads to a larger reduction of \( R_x \) in the region near the Fermi surface than in the center of the sea. Thus the electron self energies will decrease the variation of \( Q_x^{(1)} \) (contribution to \( R_x \) from diagram (1a) given in figure 3-4) across the electron sea. The task now is to make a quantitative estimate of \( Q_x(x) \) for \( x < \varphi_f \), and
of its contribution to $\Phi_{\mathbf{q}}$. From the Fourier transform of (2-13) we have that the probability of occupation function $\psi(\mathbf{q})$ is related to the Fourier transform of the electron Green's function by

$$\psi(\mathbf{q}) = i \int_{-\infty}^{\infty} d\omega e^{i\omega \mathbf{q} \cdot \mathbf{r}} \tilde{G}_e(\mathbf{q};\omega).$$  \hfill (5-1)

Further, when the positron part of the electron-positron correlation function is taken to be the free positron propagator formula (2-15) gives that $\psi(\mathbf{q})$ is related to $\Phi_{\mathbf{q}}$ simply by

$$\Phi_{\mathbf{q}} = \frac{\lambda}{V} \sum_{\mathbf{k}} \psi(\mathbf{k}) \Theta(-\mathbf{q} - \mathbf{k}) = \frac{\lambda}{V} \psi(\mathbf{q}).$$  \hfill (5-2)

The physical interpretation of this formula is obvious. It just represents a static sea of electrons with momentum distribution $\psi(\mathbf{q})$ sampled by a non-interacting positron. To calculate $\psi(\mathbf{q})$ from formula (5-1), some suitable approximation to $\psi(\mathbf{q};\omega)$ has to be chosen. This is done by examining the graphs of figure 5-1 which gives all the non-zero first order Feynman diagrams. Graphs which cancel because of the assumed fixed background of positive charge have been omitted. The diagram we wish to account for

# $\psi(\mathbf{q})$ has been calculated in the past by Daniel and Vosko.\(^{(10)}\)

Their work is based on ordinary Raleigh-Schrödinger perturbation theory and the now well known technique (first discussed by Gell-Mann and Brueckner\(^{(21)}\)) of formal summation of a certain class of terms to all orders in the perturbation series. Unfortunately, their numerical results are presented in graphical form which is not accurate enough for our purpose and we will have to recalculate these.)
is 5-lb, the first order electron self energy diagram multiplied by a free positron propagator. The contribution to $G_e(q; \omega)$ from 5-lb is given by the Fourier transform of

$$G^{(\text{lb})}(q; \gamma) = i \int \frac{d^3 \vec{q}}{2!} \frac{d^3 \vec{z}'}{2!} G_e(q; z) G_e(z; z') u(q; \varepsilon) u(z'; \varepsilon) G_e(z'; \gamma), \quad (5.3)$$

i.e.,

$$G^{(\text{lb})}(q; \omega) = \frac{i}{V} \int \frac{d^3 \vec{q}}{2!} \frac{d^3 \vec{z}'}{2!} u(q; \varepsilon) \left[ G_e^2(q; \omega) \right] G_e(q; \gamma). \quad (5.4)$$

The contribution of (5-4) to $R_q$ (or $G_e(q)$) is, using (5-1),

$$R^{(\text{lb})}_q = \frac{N}{V} \int \frac{d^3 \vec{q}}{2!} \frac{d^3 \vec{z}'}{2!} \frac{i \omega}{V} \int \frac{d^3 \vec{q}}{2!} \frac{d^3 \vec{z}'}{2!} u(q; \varepsilon) u(z'; \varepsilon) \left[ G_e^2(q; \omega) \right] G_e(q; \gamma). \quad (5.5)$$

For $p < p_f$, 

$$[G_e(q; \omega)]^2 = \Theta(p_q - p) \left[ p^2 - \omega + i\gamma \right]^2 \quad (5.6)$$

and (5-5) becomes

$$R^{(\text{lb})}_q = \frac{(i\omega)}{V^2} \int \frac{d^3 \vec{q}}{2!} \frac{d^3 \vec{z}'}{2!} \frac{i \omega}{V} \int \frac{d^3 \vec{q}}{2!} \frac{d^3 \vec{z}'}{2!} \frac{i \omega}{V} \int \frac{d^3 \vec{q}}{2!} \frac{d^3 \vec{z}'}{2!} u(q; \varepsilon) u(z'; \varepsilon) \left[ G_e^2(q; \omega) \right] G_e(q; \gamma). \quad (5.7)$$

For large $\omega$ the integrand in (5-7) behaves like $1/\omega^2$. This goes to zero sufficiently rapidly as $\omega \to \infty$ to make the contribution from a large semi-circle vanish. The exponential factor $\frac{i \omega}{V}$ is then irrelevant and can be dropped. Completing the $\omega$ contour below gives

$$R^{(\text{lb})}_q = \frac{i \omega}{V^2} \int \frac{d^3 \vec{q}}{2!} \frac{d^3 \vec{z}'}{2!} \frac{i \omega}{V} \int \frac{d^3 \vec{q}}{2!} \frac{d^3 \vec{z}'}{2!} \frac{i \omega}{V} \int \frac{d^3 \vec{q}}{2!} \frac{d^3 \vec{z}'}{2!} u(q; \varepsilon) u(z'; \varepsilon) \left[ G_e^2(q; \omega) \right] G_e(q; \gamma). \quad (5.8)$$

This integral is further reduced and evaluated in Appendix 5.
 Variation of $\bar{\mathcal{G}}_{\text{el}}^{(e)}$ and $\bar{\mathcal{G}}_{\text{ps}}^{(p)}$ with momentum ($\gamma = \phi / \rho_0$) for $\phi = 2$

These describe respectively (to first order) the effect of electron and positron self energies on $\mathcal{R}_{\phi}$.

The numerical results are shown in figure 5-3 for $\phi = 2$. The quantity $\bar{\mathcal{G}}_{\text{ps}}^{(p)}$ is of course negative, since it is proportional to the first order decrease in the occupational probability for a state inside the Fermi sphere; i.e. for $\rho_0 \phi$, $\bar{\mathcal{G}}_{\text{el}}^{(e)} = \bar{\mathcal{G}}_{\text{ps}}^{(p)}$. For sodium ($\phi = 2$) the reduction in $\bar{\mathcal{G}}_{\text{ps}}^{(p)}$ coming from $\bar{\mathcal{G}}_{\text{ps}}^{(p)}$ is about 2% of $\bar{\mathcal{G}}_{\text{el}}^{(e)}$ for $\gamma = 1$, and 8% for $\gamma = 0$. This tends to smooth out $\bar{\mathcal{G}}_{\text{ps}}^{(p)}$ as a function of $\gamma$. The positron self energy will have much the same effect.

Positron self energy.

The positron self energy effect must now be investigated. Again, because of its interaction with the surrounding medium, the positron has a spread in momentum. The positron occupational probability function $\bar{\mathcal{G}}_{\text{ps}}^{(p)}$ is not simply the theta function $\Theta(-\xi)$. Rather, it is less than 1 for $\xi = 0$ and finite for $\xi \neq 0$. From
formula (2-14), the relationship between \( G_p(k) \) and the Fourier transform of the positron correlation function is

\[
G_p(k) = i \int \frac{d\omega}{2\pi} e^{ik\omega} \mathcal{G}_p(k;\omega)
\]

(5-9)

The first order correction to \( G_p(k;\omega) \) is given by the positron part of diagram 5-1c, i.e.

\[
G^{(c)}(\omega;\omega) = i \int \frac{d^4z_1}{2\pi} U(z_1,\omega) \mathcal{G}^0_p(z_1;\omega) \mathcal{G}^0_p(z'_1;\omega) \mathcal{G}^0_p(z'_2;\omega) \mathcal{G}^0_p(z_2;\omega)
\]

(5-10)

or Fourier transforming,

\[
G^{(c)}(k;\omega) = \frac{i}{V} \sum_b \int \frac{d^4z}{2\pi} U(z,b) \mathcal{G}^0_p(k-z;\omega+\epsilon) \mathcal{G}^0_p(k-z;\omega+\epsilon) \mathcal{G}^0_p(k-z;\omega+\epsilon) \mathcal{G}^0_p(k-z;\omega+\epsilon)
\]

(5-11)

Denote the contribution of (5-11) to \( G_p(k) \) by \( \mathcal{G}^{(c)}_p(k) \); then

\[
\mathcal{G}^{(c)}_p(k) = \frac{i}{V} \sum_b \int \frac{d^4z}{2\pi} U(z,b) \int \frac{d\omega}{2\pi} \mathcal{G}^0_p(k-z;\omega) \mathcal{G}^0_p(k-z;\omega) \mathcal{G}^0_p(k-z;\omega) \mathcal{G}^0_p(k-z;\omega) \left[ \frac{\Theta(-k)}{(k^2-\omega+\epsilon)^2} + \frac{\Theta(k)}{(k^2+\omega-\epsilon)^2} \right]
\]

(5-12)

The \( \omega \) integration in (5-12) can be done by completing the contour below for the \( \Theta(-k) \) term, and above for the \( \Theta(k) \) term. Thus (5-12) can be rewritten as

\[
\mathcal{G}^{(c)}_p(k) = \Theta(-k) \frac{i}{V} \int \frac{d^4z}{2\pi} U(z,b) \left[ \frac{-\Theta(1-k-z)}{(k^2-\omega+\epsilon)^2} - \frac{\Theta(-k-z)}{(k^2-\omega-\epsilon+\epsilon)^2} \right] + \Theta(k) \left[ \frac{i}{V} \int \frac{d^4z}{2\pi} U(z,b) \frac{-\Theta(-k-z)}{(k^2-\omega-\epsilon)^2} \right]
\]

(5-13)

The first term in (5-13) just gives the decrease in the probability of finding the positron in a state \( |\kappa\rangle \) while the second gives the probability of finding the positron in a state \( |\kappa+\rangle \). Now \( \mathcal{G}^{(c)}_p(k) \) describes only the positron part of diagram 5-1c. The electron
part is the free electron propagator \( G(x, y) \) which corresponds to \( G_{\phi}(\xi, \phi(x, y)) \). Thus from formula (2-15), the contribution of diagram 5-1c to \( g_{\phi} \) can be written as

\[
R_{\phi}^{(c)} = \frac{\lambda}{V} \theta(k - p) \left[ \frac{\Delta \xi}{2\pi} \right] \int \frac{d\xi}{\xi + \eta} \left( \frac{\Theta(k - p - i\xi)}{(-\xi^2 - \epsilon + i\eta)^2} \right)
\]

\[
+ \frac{\lambda}{V} \left[ \frac{\Delta \xi}{2\pi} \right] \int \frac{d\xi}{\xi + \eta} \left( \frac{\Theta(k - p - i\xi)}{(-\xi^2 - \epsilon - i\eta)^2} \right).
\]

The physical interpretation of equation (5-14) is straightforward. The first term is just the Sommerfeld partial annihilation rate \( Q_{\phi}^{(a)} \) multiplied by \( G_{\phi}^{(c)} \), the first order decrease in the probability of finding the positron in the state \( \langle x \rangle \). This contribution is negative. The second term describes the sampling of a non-interacting sea of electrons by a free positron in a state \( \langle x \rangle \), multiplied by the probability \( \Theta_{\phi}(x, y) \) of the positron actually having momentum \( x \), and summed over all possible states \( \langle x \rangle \); i.e., it can be written as

\[
\frac{\lambda}{V} \int_{k + 0} \theta(k - x, y) G_{\phi}(x) \cdot
\]

Note that (5-15) is a positive contribution and is non-zero for both \( p > p_r \) and \( p < p_r \). For \( p > p_r \), equation (5-14) can be rewritten as

\[
R_{\phi}^{(c)} = \frac{\lambda}{V^2} \left[ \frac{\Delta \xi}{2\pi} \right] \int \frac{d\xi}{\xi + \eta} \left( \frac{1}{(-\xi^2 - \epsilon + i\eta)^2} - \frac{\Theta(k - x, y)}{(-\xi^2 - \epsilon - i\eta)^2} \right).
\]

For the numerical evaluation of this integral, see Appendix 5.

The results are presented graphically in figure 5-3 for \( d = 2 \).

This again amounts to a reduction of \( Q_{\phi}^{(a)} \) with the reduction increasing as \( x \) increases from 0 to \( p_r \). Finally, the quantity of interest \( \bar{R}_{\phi}^{(c)} + \bar{R}_{\phi}^{(b)} + \bar{R}_{\phi}^{(a)} \) is shown in figure 5-4 for \( d = 2 \).
Variation with momentum of $\bar{\mathcal{R}}^{\text{(1)}}_{\nu \nu} + \bar{\mathcal{R}}^{\text{(1)}}_{\pi \pi} + \bar{\mathcal{R}}^{\text{(1)}}_{\mu \mu}$ i.e. $\bar{\mathcal{R}}^<_{\nu \nu}$ from the first order ladder, electron self energy, and positron self energy diagrams. Also plotted for comparison is $\bar{\mathcal{R}}^{\text{(1)}}_{\nu \nu}$ and $\bar{\mathcal{R}}^{\text{(1)}}_{\mu \mu} + \bar{\mathcal{R}}^{\text{(1)}}_{\nu \nu}$. Its variation across the sea from $\nu = 1$ to $\nu = 9$ has been reduced to about 14%. Also shown in figure 5-4 for comparison is $\bar{\mathcal{R}}^{\text{(1)}}_{\nu \nu}$ and $\bar{\mathcal{R}}^{\text{(1)}}_{\mu \mu} + \bar{\mathcal{R}}^{\text{(1)}}_{\nu \nu}$. It appears that Kahana's static potential is even more appropriate to describe the variation of $\mathcal{R}$ across the Fermi sea than was originally expected in the sense that approximating the dynamic potential in $\mathcal{R}^{\text{(1)}}_{\nu \nu}$ by its static limit and correcting for the plasmon has very much the same effect as including self energies. To get an idea of how near this equivalence is, write $\bar{\mathcal{R}}^{\text{(1)} \cdot \text{(1)} \cdot \text{(1)} \cdot \text{(1)}}_{\nu \nu}$ as $1.972 + 0.261 \nu^2 + 0.089 \nu^4$; this leads to a total annihilation rate of $2.186 \mathcal{R}^\ast = \mathcal{R}^{\text{(1)} \cdot \text{(1)} \cdot \text{(1)} \cdot \text{(1)}}_{\nu \nu}$. But from Chapter 3 we have $\mathcal{R}^\ast = 1.911 \mathcal{R}^\ast$ and $\mathcal{R}^{\text{(1)} \cdot \text{(1)} \cdot \text{(1)} \cdot \text{(1)}}_{\nu \nu} = 0.34$. Therefore $\mathcal{R}^\ast \cdot \mathcal{R}^\ast = 2.25 \mathcal{R}^\ast$, which agrees with $\mathcal{R}^{\text{(1)} \cdot \text{(1)} \cdot \text{(1)} \cdot \text{(1)}}_{\nu \nu}$ to within 3%.

Finally, it is worth noting that $\mathcal{R}^{\text{(1)} \cdot \text{(1)} \cdot \text{(1)} \cdot \text{(1)}}_{\nu \nu}$ is indistinguishable from $\mathcal{R}^{\text{(1)}}_{\nu \nu} = 2.19 \mathcal{R}^\ast$. Hence $\mathcal{R}^{\text{(1)} \cdot \text{(1)} \cdot \text{(1)} \cdot \text{(1)}}_{\nu \nu} \approx \mathcal{R}^{\text{(1)}}_{\nu \nu}$.
since \( A_2^{(1)} + A_2^{(2)} = 0 \) and \( A_2^{(1)} + A_2^{(2)} = 0 \). Thus \( A_2^{(1)} + A_2^{(2)} + A_2^{(3)} = 0 \).

In the next chapter we will actually look at \( A_2^{(1)} \), \( A_2^{(2)} \), and \( A_2^{(3)} \) in detail, and arrive at the conclusion that their sum is almost zero. This is an excellent check on our numerical work.
Chapter 6

EFFECTIVENESS OF ELECTRON-ELECTRON INTERACTIONS AT PRODUCING TAILS IN THE ANGULAR DISTRIBUTION CURVE

Introduction.

The probability of occupation $\mathcal{Q}_\rho(\phi)$ of a state $|\rho,\phi\rangle$ by an electron in a fully interacting electron gas is given in figure 5-2 to first order in the perturbation series (diagram 5-1b). There is a discontinuity in $\mathcal{Q}_\rho(\phi)$ at $\rho > \rho_*$ but not a sharp cut-off. Thus there is a probability of finding an electron in a state of momentum $\rho$ with $\rho > \rho_*$. Since the angular distribution of the annihilation gamma-rays is in some sense a measure of the momentum distribution in the metal, a question immediately arises: Are the tails resulting from the presence of electrons with momentum greater than $\rho_*$ large enough to show up in the angular correlation curve? To answer this question it is convenient to proceed in two steps. First the positron force is neglected and the tails coming from $\mathcal{Q}_\rho(\phi)$ are computed and compared with the experimental results for sodium. Secondly, the positron is allowed to interact, and the resulting distortion introduced into the system is investigated. The theory is first set up for a high density gas and then an attempt is made to extend it to lower densities using an analogy with the work of K-II. The results can be summarized as follows. When the positron force is neglected, the partial annihilation rate $\mathcal{Q}_\rho$ is proportional to $\mathcal{Q}_\rho(\phi)$ and the tails introduced in the gamma-ray angular correlation curve from diagram 5-1b are short (of the order $\rho_*$) but quite considerable; they would certainly show up experimentally. When the positron is allowed to interact, this simple picture breaks down completely.
The reason for the breakdown is that as soon as the positron force is included, there are many other diagrams of the same order as 5-lb which contribute to $\mathcal{Q}_\Phi$ for $\Phi \rightarrow \Phi$. First note that the lowest order contribution to $\mathcal{Q}_\Phi(\Phi)$ from 5-lb is really of second order as shown in figure 6-lb. To see this we need only notice that replacing the full dynamic potential in 5-lb by some static equivalent gives zero for $\mathcal{Q}_\Phi(\Phi)$. Four other diagrams contributing to $\mathcal{Q}_\Phi$ are

1) from Chapter 3 (Chapter 5), the first order ladder (positron self energy) graph with full dynamic potential; its lowest order contribution is 6-la (6-lc).

2) from Chapter 4, the two second order graphs 4-la and 4-lc representing the possibility of particle-hole interactions.

There is one more second order graph that should be mentioned. It is the second order electron self energy exchange diagram 1-3 (12) which represents a correction to 5-lb. Its contribution to $\mathcal{Q}_\Phi(\Phi)$ is negative but quite small (roughly a factor of 10 smaller than that from 5-lb).

This accounts for all the second order graphs in the expansion of the electron-positron correlation function except for those of group 1 as defined in Chapter 4. However, these correspond to enhancement effects and will be taken up in the second part of this chapter.

**Figure 6-1**

![Diagrams](image)

Lowest order contribution to $\mathcal{Q}_\Phi$ from diagrams 5-la, 5-lb and 5-lc.
Now what do all these diagrams mean? To begin, consider the positron self energy case. Due to its interaction with the surrounding medium, there is a probability of finding the positron in a state $|\nu\nu\rangle$. This positron can then sample the sea of non-interacting electrons, leading to a positive contribution to $Q_\nu$ of the same order of magnitude as that from electron self energies. This is the simplest modification introduced by the positron force.

Next note that whenever an electron is above the sea, there must be in the passive electron sea at least one hole and another hole-particle pair (unless of course the electron should be there by virtue of a first coulomb correlation with the positron, in which case there would be only a hole in the electron sea). In other words, in ordinary space an electron with momentum $p>\rho$ necessarily implies that there is a charge disturbance in its neighbourhood. But the incoming positron can then correlate with this charge disturbance. This is partially accounted for by the ladder graph 5-la. For $p<\rho$, this graph represents a screened monopole interaction between annihilating electron-positron pair, but for $p>\rho$, it represents a screened dipole interaction. That is, in this case there is no direct interaction between annihilating electron-positron pair, but only between the positron and the screening charge (hole-particle pair) around it.* This polarization diagram 5-la contributes a negative amount to $Q_\nu$ and is large enough to cancel out almost completely the combined effect of 5-lb and 5-lc.

*(Note that in this section we could just as well have talked about a positron with $\nu\nu$ being sampled by an incoming electron.)
When the first interaction (in the sense of perturbation theory) is an electron-positron interaction, there is further the possibility in second order of correlation of either the positron or the electron with the hole left behind in the passive sea by the excited electron. This has been discussed in some detail in Chapter 4. The electron hole -positron interaction diagram 4-lb leads to a reduction of $Q_q$ (denote it by $Q_q^{\text{ph}}$), but in magnitude it is roughly a factor of 10 smaller than the contribution to $Q_q$ from electron self energies. On the other hand, the electron hole -electron interaction leads to a positive contribution to $Q_q$. It is as large as $Q_q^{\text{ph}}$ plus the correction to $Q_q$ from 1-3 (12). Thus not only would each of these contributions introduce almost negligible tails, but further, one carries a positive sign while the others both carry negative signs, with the net result that they cancel. Thus we are left with the conclusion that once the positron force is taken seriously, the tails found from electron self energies disappear. This completes the high density theory.

We next turn to enhancement effects, i.e. to the possibility of the annihilating electron-positron pair interacting with each other once they are, so to speak, above the sea. To do this we must take account of the diagrams of group 1 of Chapter 4. However, proceeding by analogy with the work of K-II, we are led to consider many other higher order graphs which form a more natural group. This work will be done only for diagrams 5-la,-lb and -lo, since the hole-particle interaction contributions are small anyway. As can be expected, our calculation indicates that the cancellation between these three graphs remains even when the enhancement effects are included.
Electron self energies.

To get an idea of how the real momentum distribution in a fully interacting electron gas can affect the angular correlation curve for $e \cong e_\nu$, the simplest approximation is to neglect the positron force entirely. This is at best a first step, since the positron coulomb field is known to introduce important correlations into the problem. However, this approximation should give some idea of how the angular distribution of the gamma-rays is modified and perhaps give a rough order of magnitude for the "tails" that can be expected for positron annihilation in a fully interacting valence gas.

When the positron force is neglected, the partial annihilation rate $\tilde{Q}_p$ is simply given by $\tilde{Q}_p = \lambda \tilde{Q}_p(\omega)$, where $\tilde{Q}_p(\omega)$ is the probability of occupation of a state of momentum $\omega$ by one of the valence electrons. The contribution to $\tilde{Q}_p$ from the first order electron self energy diagram 5.1b is given by formula (5-5). Since for $\omega > \omega_c$, $[\tilde{Q}_p(\omega)]^2 = \omega(\omega - \omega_c)/[\omega^2 - (\omega - \omega_c)]^2$, (5-5) gives that

\[
\tilde{Q}_p^{(1)}(\omega) = \frac{(i\lambda)^2}{\sqrt{2}} \left\langle \frac{d\omega}{2\pi} \frac{d\omega}{2\pi} \frac{i\omega\omega_c}{\omega^2 - (\omega - \omega_c)^2} \right\rangle C_0(\omega - \omega_c, \omega - \omega_c).
\]

This expression is easily reduced to a double integral and evaluated numerically. The results are tabulated in Appendix 6 and shown graphically in figure 6-2. However, the measured quantity is not $\tilde{Q}_p$ but $\tilde{Q}_p^{\text{obs}}$, which is related to $\tilde{Q}_p$ by

\[
\tilde{Q}_p^{\text{obs}} = \int_{\frac{1}{2}}^\infty \tilde{Q}_p^{(1)}(\omega) \, d\omega \, d\theta \, \frac{3}{2} \, \tilde{Q}_p^{\text{c}}.
\]
The quantities \( \delta_{\text{e}}^{1 \text{b}} \) and \( \delta_{\text{p}}^{1 \text{c}} \), give respectively the contribution to \( Q_\gamma \) from electron and positron self energies in first order perturbation theory (diagrams 5-1b and 5-1c) for \( \gamma > 1 \); \( Q_{\text{p}}^{1 \text{b}} \) is a similar contribution from the polarization graph 5-1a. These curves are for \( \alpha = 0.2 \), i.e. \( \alpha_\gamma = 3.78 \).

From the tabulated values of \( \delta_{\text{e}}^{1 \text{b}} \), integral (6-2) can be evaluated for fixed \( \gamma > 1 \). The results are shown in figure 6-3a; for fixed reference the Sommerfeld inverted parabola has also been plotted. Although the tails that result are short (they do not extend beyond \( 2 \alpha_\gamma \)), they are appreciable and if real would certainly appear experimentally. The experimental results of A.T. Stewart for sodium are given in figure 6-3b; \( Q(\varphi) \) is the two-photon counting rate in arbitrary units and \( \varphi \) is the angle between the photon pair, related to \( \gamma \) through the equation \( \varphi = \left( \frac{1.88}{\pi} \right) \gamma \). If the very long and broad tail, through the points of which a solid line has
The angular correlation curve when self energy effects are included to first order (diagram 5-1b).

been drawn, is tentatively ascribed to core annihilation (this will be justified in Chapter 7), there still remain around \( \varphi > \varphi_F \) ( \( e > e_F \) ) some events corresponding to the annihilation of a pair having momentum greater than the Fermi momentum. Reference to the theoretical curve of 6-3a would indicate that these events could very well come from electron-electron interactions. The shape of the theoretical curve certainly appears correct although it seems a little too large. However it must be stressed that part of this "smearing" is definitely due to the instrument resolution; how much is difficult to estimate accurately. Stewart, in his paper
Stewart's experimental results for the angular correlation of the annihilation gamma-rays for sodium. The angle $\theta_c$ is the cut-off angle of the Sommerfeld theory.

on the Fermi surface of sodium, claims that once this instrument resolution is "subtracted out" there still remains appreciable "smearing". It seems worth while to pursue the calculation further and try to answer the following questions:

1. To what extent do higher order electron self energy diagrams affect the momentum distribution function?

2. How much does the positron force change the results of figure 6-3a?
Higher electron self energy diagrams.

All the electron self energy diagrams which need to be considered up to second order are shown in figure 6-4. Of the three second order Feynman graphs shown in this figure we have up to now accounted for only one, (e). The contributions from (c) and (d) to the electron propagator \( G_e(x,y) \) are respectively

\[
G_e^{ac}(x,y) = \langle i \rangle \int d^4 x_1 d^4 x_2 d^4 x_3 d^4 x_4 \, \delta^4(x-x_1) \delta^4(x_1-x_2) \delta^4(x_2-x_3) \delta^4(x_3-x_4) \, G_e(x_3,y) G_e(x_4,y) x 
\]

\[
G_e^{de}(x,y) = \langle i \rangle \int d^4 x_1 d^4 x_2 d^4 x_3 d^4 x_4 \, \delta^4(x-x_1) \delta^4(x_1-x_2) \delta^4(x_2-x_3) \delta^4(x_3-x_4) \, G_e(x_3,y) G_e(x_4,y) x 
\]

and

Fourier transforming these equations, they become

\[
G_e^{ac}(k,\omega) = \langle i \rangle \int \frac{d^4k}{(2\pi)^4} \frac{d^4\omega}{(2\pi)^4} \, G_e^0(k,\omega) G_e^0(k,\omega) x 
\]

\[
G_e^{de}(k,\omega) = \langle i \rangle \int \frac{d^4k}{(2\pi)^4} \frac{d^4\omega}{(2\pi)^4} \, G_e^0(k,\omega) G_e^0(k,\omega) x 
\]

Figure 6-4

Electron propagator to second order in the perturbation theory.
Observe that the \( \omega \) dependence of \( \mathcal{G}_e^r(k;\omega) \) is all contained in the factor \( [\mathcal{G}^r(k;\omega)]^2 \); hence when \( \mathcal{G}_e^r(k;\omega) \) is integrated over \( \omega \) (as is required in order to get the contribution to \( \mathcal{Q}_e(k) \) from \( \mathcal{G}_e^r(k;\omega) \)) the integral vanishes. More explicitly, for \( k > k_F \) (\( k < k_F \)) the integrand has no singularities in the upper (lower) half plane so that closing the contour above (below) gives zero.

The contribution from \( \mathcal{G}_e^{rd}(k;\omega) \) to the probability of occupation function \( \mathcal{Q}_e(k) \) does not vanish. It is

\[
\mathcal{P}_e^{rd}(k) = \frac{e^{i\beta}}{V^2} \prod_{(k^{\ast})} \left\{ \int \frac{d\epsilon d\epsilon'}{2\pi} \left[ \mathcal{G}_e^0(k;\omega) \right]^2 \mathcal{G}_e^r(k+q;z;\epsilon+\epsilon'-\omega) \right\} \mathcal{G}_e^0(k-q;z;\epsilon') \mathcal{G}_e^0(k+q;z;\epsilon') \tag{6.6}
\]

Concentrate on the region \( k > k_F \). In this case the only singularity of the integrand in the upper \( \omega \)-plane is the simple pole at \( \omega = -(k^2+q^2)^{1/2} + \epsilon + \epsilon' + i\eta \), coming from the propagator \( \mathcal{G}_e^r(k+q;z;\epsilon+\epsilon'\omega) \). Closing the contour above gives

\[
\mathcal{P}_e^{rd}(k) = \frac{e^{i\beta}}{V^2} \prod_{(k^{\ast})} \left\{ \int \frac{d\epsilon d\epsilon'}{2\pi} \left[ \mathcal{G}_e^r(k;\omega) \right]^2 \mathcal{G}_e^0(k-q;z;\epsilon') \mathcal{G}_e^0(k+q;z;\epsilon') \right\}. \tag{6.6}
\]

The \( \epsilon \) and \( \epsilon' \) integrations must now be done. This is a simple matter. No special advantage is gained by doing one first rather than the other, and the result is

\[
\mathcal{P}_e^{rd}(k) = -\frac{1}{V^2} \prod_{(k^{\ast})} \mathcal{N}_e \mathcal{N}_e' \frac{\Theta(k_F-k_F')\Theta(k_F-k^2-k^2)\Theta(k_F-k^2-k^2)\Theta(k^2-k^2)}{\left[ k^2 + (k+q)^2 - (k-F)^2 - (k+q)^2 - i\eta \right]^2}. \tag{6.7}
\]

The "\( i\eta \)" factor can be dropped. A Monte Carlo method was used for the numerical evaluation of this integral which is discussed
in Appendix 6. This contribution is negative but reduces only slightly the tails found in the first part of this chapter. This completes our discussion of the momentum distribution in an interacting electron gas and its effectiveness in producing tails.

**Positron self energy.**

We must now investigate what modification is introduced into the theory when the positron force is taken into account. The situation is now considerably complicated in the sense that many additional processes of the same order occur; these have been surveyed in the introduction. Perhaps the simplest modification that arises is that, although the positron is thermalized, it is not in a simple plane wave state of zero momentum. Because of its interaction with the surrounding medium there is a probability of finding the positron in a state with momentum different from zero. That is, positron self energy effects have to be considered. Formulae (5-15) and (5-14) give that the contribution to \( R_p \) from the first order positron self energy diagram multiplied by a free electron propagator can be written as

\[
\mathcal{G}_p^{(\xi)}(\xi) = \frac{1}{V} \sum_{\xi \geq 0} \Theta(p_x - \xi - \xi_0) \mathcal{G}_p^{(\xi)}(\xi)
\]

\[
= \frac{V^2}{\xi} \sum_{\xi_0} \Theta(p_x - \xi - \xi_0) \int_{q+\xi} \frac{d\xi}{2\pi} \frac{u_0(q, \xi)}{(6 - z - z_0 - \xi)^2}
\]

(5-8)

The expression \( \mathcal{G}_p^{(\xi)}(\xi) \) is just the probability of finding the positron in a state of momentum \( \xi \) with \( \xi \geq 0 \) in first order perturbation theory. The theta function \( \Theta(p_x - \xi - \xi_0) \) is the probability of finding an electron in a state of momentum \( p_x - \xi \) in zeroth order perturbation theory. Hence except for a multiplicative factor, \( \mathcal{G}_p^{(\xi)}(\xi) \) is just the product of these two occupational probabilities.
summed over all possible positron momenta \( \kappa \). To get a quantitative estimate of the effect of this process on the angular correlation curve, equation (6-8) has to be reduced to a more manageable form. For details see Appendix 6. The results are presented graphically in figure 6-2, which indicates that positron self energies are slightly more effective at producing "tails" than electron self energies.

**First order ladder graph.**

Consider an electron above the Fermi sea. Suppose it was promoted there because of its interaction with another valence electron. Then, besides the hole left behind in the sea by the given electron, there must be present in the system (because of momentum conservation and the Pauli Principle) another electron hole-particle pair. In other words, in the lowest approximation the presence of an electron above the sea is always accompanied by the existence of a charge disturbance in its immediate vicinity. (This is in contrast with the case of an electron below the Fermi sea, which in lowest approximation is in a region of charge neutrality.) Now clearly it is possible for the incoming positron to interact with this charge disturbance. Diagram 6-la accounts partially for this possibility. It represents a process in which the incoming positron interacts with a hole-particle pair present in the system because of a previous electron-electron interaction. This diagram is in fact the lowest order contribution to \( Q_e \) for \( \rho \). coming from the polarization graph 5-la. This is so because for \( \rho \), the first order ladder graph with static potential does not contribute to \( Q_e \). Thus diagram 5-la for \( \rho \) represents a screened dipole interaction between the positron and the hole-particle pair around the electron. Note that the physical inter-
pretation of 5-la for $p \varphi_\rho$ is quite different. In this case it is possible to have a direct interaction between the annihilating electron-positron pair, and 5-la thus describes a screened monopole interaction.

From formula (3-10), $Q^{(18)}_\rho$ from diagram 5-la is given by

$$Q^{(18)}_\rho = \lambda \left( \frac{\omega}{\kappa} \right)^2 \frac{\omega(\omega - \kappa)}{\kappa^2 - \omega - i\eta} \overline{\rho}^{(\omega - \kappa, \omega)} \frac{1}{\rho^2 - (\omega - \kappa)^2 - \omega - i\eta}.$$  \hspace{1cm} (6-1)

The "polarization charge" around the electron of course tends to keep the positron away and so $Q^{(18)}_\rho$ must be negative. For the numerical evaluation of $Q^{(18)}_\rho$, see Appendix 6; the results are presented in figure 6-2. $Q^{(18)}_\rho$ is negative and large enough to cancel out almost completely the tails coming from both the electron and the positron self energy effects; in fact, the remainder is quite negligible. It would seem then that the positron is effectively kept away from an electron with momentum $p \varphi_\rho$. Note that in this section we have chosen to discuss the case of an electron above the sea which we then try to sample with a thermalized positron. We could just as well have considered a positron with momentum $\varphi_{\rho \omega}$ (and hence with screening charge around it) which is sampled by a sea electron; diagram 6-la would again represent the

**Figure 6-5**

The specific time ordering of diagram 6-la which leads to a contribution to $Q_\rho$ with $p \varphi_\rho$. The double horizontal line at time $t$ represents the action of the "annihilation operator".
interaction of the annihilating electron with the charge disturbance around the positron.

To conclude this section we draw attention to diagram 6-5. It results from 6-la when 6-la is analysed in terms of "time independent perturbation theory" type contributions, and only that part corresponding to annihilation with the emission of momentum \( \mathbf{q} \) is retained. The annihilation process is explicitly represented. This term is an interference term in the sense that the wave function on the right hand side of the "annihilation operator" is different from that on the left hand side. A similar analysis could be given for the electron and the positron self energy diagrams but little can be learned from this so we will not carry the discussion further.

Hole-particle interactions.

There are two other second order processes contributing to \( \Phi_\pi \) for \( \mathbf{q} \), which must now be considered. They correspond to the possibility of hole-particle interactions and have been discussed in detail in Chapter 4. To summarize briefly, consider an electron knocked above the Fermi sea due to its interaction with the positron. There is then a possibility that either the excited electron or positron can correlate with the hole left behind by the given electron. Such processes are possible in second order perturbation theory and are shown in diagrams 4-1b and 4-1c. Their contributions to \( \Phi_\pi \) have already been written down in Chapter 4. Formula (4-8) gives that positron -electron hole interactions contribute

\[
\Phi_{\pi, e-h}^\pi = -\frac{\lambda^2}{V^2} \sum_{\mathbf{q}, \mathbf{k}} U(\mathbf{q}, \mathbf{0}) U(\mathbf{k}, \mathbf{0}) \frac{\delta(\mathbf{p}_e + \mathbf{p}_h - \mathbf{p}_e - \mathbf{p}_h) \delta(\mathbf{p}_e + \mathbf{p}_h - \mathbf{p}_e - \mathbf{p}_h)}{[(\mathbf{q} + \mathbf{k})^2 - \mathbf{q}^2 - (\mathbf{p}_e - \mathbf{p}_h)^2][(\mathbf{q} - \mathbf{k})^2 - \mathbf{q}^2 - (\mathbf{p}_e + \mathbf{p}_h)^2} \tag{6-10}
\]
which is negative, while formula (4-24) gives that the contribution of electron-electron hole interactions is

\[
\hat{\theta}_{e-e}^e = \sum_{\sigma} \frac{2 \theta(p_{e} - q_{e} + q_{e}) \theta(q_{e} - q_{e} - p_{e}) \theta(p_{e} - q_{e} + q_{e})}{b_{e} q_{e} \left[ q_{e}^{4} - (q_{e} - q_{e})^{4} + (q_{e} - q_{e})^{2} \right] \left[ p_{e}^{2} - (q_{e} - q_{e})^{2} + (q_{e} - q_{e})^{4} \right]}
\]

which is positive. For the numerical evaluation of these integrals see Appendix 6. It is to be noted that both \(\hat{\theta}_{e-e}^e\) and \(\hat{\theta}_{p-p}^e\) in absolute value are of the order 10 smaller than \(\theta_{e-e}^e\), and their sum adds approximately the same amount to the "tails" as we subtracted away by including \(\theta_{e-e}^e\) (the second order electron self energy exchange diagram). At this point we are forced to the rather amazing conclusion that in a fully interacting electron gas there are no significant "tails" in the gamma-ray angular correlation curve.

Our theory so far can be considered a high density theory. We now turn to the problem of enhancement effects, i.e. we take into account the electron-positron force once the annihilating pair is excited above the sea. Since the contributions from the two hole-particle interaction diagrams are individually quite small, we will develop the theory only for the three diagrams 5-1a, -1b and -1c.
Enhancement effects.

We have not as yet considered enhancement effects. For instance take the case of electron self energies. Because of its interaction with the surrounding medium there is a probability for an electron to be knocked above the Fermi sea and then be annihilated with the zero momentum positron. But in this simple process the attractive force between the annihilating pair is not included. This attraction could increase considerably the electron density at the positron. To take account of this enhancement effect it is clear that we must sum, at least in some approximation, the entire set of ladder diagrams with self energy effects included in the electron lines. Proceeding by analogy with the theory of K-II, the type of thing we would like is to write the contribution to $Q_p$ from all these ladder graphs in the form

$$ R_p = \sum Q(p) \cdot \xi(p) $$(6.11)

where $\xi(p)$ is an enhancement factor given by the square of some Bethe-Goldstone amplitude. This amplitude is to describe adequately the modifications in the wave function of the annihilating pair due to their interaction once they are so to speak above the sea. It is not obvious a priori that the program just outlined can actually be carried out in detail. Physically it seems reasonable, and should at least serve as a guide to the correct picture. In fact, as we proceed it will become apparent that this rather simple model has a great deal of validity and requires only slight modifications.
Formal manipulations. *

To be completely general we begin by writing down the integral equation for the sum of all ladder diagrams with self energy effects included in all electron and positron lines. That is, write

\[ G_{\Phi}(\pi\alpha'\gamma';\pi\gamma) = C_\Phi(\pi\gamma) G_{\Phi}(\pi\alpha'\gamma') - i \int \frac{d^3 \mathbf{q}}{(2\pi)^3} G(\pi\alpha';\pi\gamma) C_\Phi(\pi\gamma) G_{\Phi}(\pi\alpha'\gamma') G_{\Phi}(\pi\gamma) \]  

(6-13)

where the static limit of the effective potential \( u(q,0) \) replaces the simple coulomb law. As was done in Appendix 3, a Bethe-Goldstone amplitude \( \Lambda \) can be introduced and the equation (6-13) replaced with an equation for \( \Lambda \). The only difference between the present situation and that in Appendix 3 is that all free one-particle propagators are now to be replaced by the full propagators. But the manipulations of Appendix 3 up to equation (A3-8) are independent of the actual form of the one-particle propagators. Thus from equations (A3-7) and (A3-8) we have

\[ \Lambda_{\mathbf{m} \mathbf{m}'\mathbf{m}'} = S_{\mathbf{m} \mathbf{m}'} S_{\mathbf{m} \mathbf{m}'} + \frac{i}{\hbar} \sum_{\mathbf{q}} u(q, \omega) \int \frac{d\omega'}{(2\pi)^3} C_{\mathbf{m} \mathbf{m}'} G_{\mathbf{m} \mathbf{m}'} \Lambda_{\mathbf{m} \mathbf{m}'\mathbf{m}'} \]  

(6-19)

and

\[ \Phi_{\mathbf{m} \mathbf{m}'} = -\frac{1}{\hbar} \sum_{\mathbf{m} \mathbf{m}'} S_{\mathbf{m} \mathbf{m}'} S_{\mathbf{m} \mathbf{m}'} \int \frac{d\omega'}{(2\pi)^3} \Lambda_{\mathbf{m} \mathbf{m}'\mathbf{m}'} \left( \frac{d\omega}{2\pi} \right) C_{\mathbf{m} \mathbf{m}'} G_{\mathbf{m} \mathbf{m}'} \Phi_{\mathbf{m} \mathbf{m}'} \]  

(6-18)

*(This section is quite technical in nature and the material presented in it could very well have been put in an appendix. For the convenience of the reader the main results are summarized on page 109. Very little is lost in the continuity of the presentation by passing immediately to this summary.)
Introducing a matrix notation, equations (6-14) and (6-15) can be replaced by the formal relations

\[ <\omega m | \Sigma(\omega) = 1 + G_e G_p u | \omega m'> \]  

(6-16)

and

\[ A_{\omega} = -\frac{1}{\sqrt{V}} \sum_{m, m'} S_{\omega m} e^{i \omega \tau} \int \frac{dm}{2\pi} \frac{e^{i \omega \phi}}{i <m, m | \Sigma(\omega) G_e G_p | m', m'>} \]  

(6-17)

where, for example,

\[ <\omega m | G_e G_p | m', m''> = \sum_{m} \sum_{m'} \left( \frac{de}{d\phi} \right)^{\frac{1}{2}} G_e(m' \phi) G_p(m' \phi - \omega \phi) \]  

(6-12)

If the iterated solution, of equation (6-16) is introduced into the expression \( \Sigma G_e G_p \), the \( n \)'th order term in its expansion is

\[ G_e G_p \cdot \cdot \cdot G_e G_p \cdot \cdot \cdot | m, m' > \]  

(6-14)

Now make the following approximation in (6-19). Keep \( G_e \) to first order and replace all other propagators by their free value. This leads to \( m+1 \) terms, namely

\[ G_e G_p \cdot \cdot \cdot G_e G_p \cdot \cdot \cdot | m, m' > \]  

(6-20)

However, (6-20) is just the \( n \)'th order contribution in the expansion of \( \Sigma G_e G_p \), where by definition

\[ \Sigma^0 = 1 + G_e G_p u \]  

(6-21)

\[ \Sigma^{n+1} = 1 + \Sigma^0 u + G_e G_p \]  

(6-21)
Hence in the approximation where electron self energies are kept to first order in one line and to zeroth order in all others, \( \Sigma_{e \rightarrow p} \) can be replaced by \( \Sigma_{e \rightarrow p} \Sigma_{p \rightarrow e} \). Thus equations (6-14) and (6-15) can be replaced by

\[
\Sigma^{e \rightarrow p}_{m,n \rightarrow m',n'}(\omega) = \frac{\delta(m-n)\delta(n)}{m^2 + m^2 - \omega^2 - i \delta} \frac{1}{\Gamma^2} \int d\nu \Delta_{m,n} \Sigma^{e \rightarrow p}_{m,n} \Sigma^{p \rightarrow e}_{m',n'}(\omega)
\]

(6-22)

\[
\Sigma^{p \rightarrow e}_{m,n \rightarrow m',n'}(\omega) = \frac{\delta(m-1,m)\delta(n)}{m^2 + m^2 - \omega^2 - i \delta} \frac{1}{\Gamma^2} \int d\nu \Delta_{m,n} \Sigma^{p \rightarrow e}_{m,n} \Sigma^{e \rightarrow p}_{m',n'}(\omega)
\]

(6-23)

\[
\rho_f = -\frac{1}{\Gamma} \sum_{m,n} \sum_{m',n'} \left\{ \sum_{\nu} \frac{i}{\omega - \nu} \Delta_{m',n'} \right\} \Delta_{m,n} \sum_{\nu} \frac{i}{\omega - \nu} \Delta_{m',n'} \sum_{\nu} \frac{i}{\omega - \nu} \Delta_{m,n} \sum_{\nu} \frac{i}{\omega - \nu} \Delta_{m',n'}
\]

(6-24)

Now for \( m + n = \frac{1}{4} \) and \( m' + n' = \frac{1}{4} \) the theta function products \( \Theta(\nu - m)\Theta(-n) \) in (6-22) and \( \Theta(\nu - m')\Theta(-n') \) in (6-23) reduce to \( \rho \rho_f \). But we are interested here only in the case \( \rho > \rho_f \); hence the second term in both (6-22) and (6-23) can be dropped, giving

\[
\Sigma^{e \rightarrow p}_{m,n \rightarrow m',n'}(\omega) = \frac{\delta(m-n)\delta(n)}{m^2 + m^2 - \omega^2 - i \delta} \frac{1}{\Gamma^2} \int d\nu \Delta_{m,n} \Sigma^{e \rightarrow p}_{m,n} \Sigma^{p \rightarrow e}_{m',n'}(\omega)
\]

(6-25)

\[
\Sigma^{p \rightarrow e}_{m,n \rightarrow m',n'}(\omega) = \frac{\delta(m-1,m)\delta(n)}{m^2 + m^2 - \omega^2 - i \delta} \frac{1}{\Gamma^2} \int d\nu \Delta_{m,n} \Sigma^{p \rightarrow e}_{m,n} \Sigma^{e \rightarrow p}_{m',n'}(\omega)
\]

(6-26)

Rewrite (6-24) as

\[
\rho_f = -\frac{1}{\Gamma} \sum_{m,n} \sum_{m',n'} \left\{ \sum_{\nu} \frac{i}{\omega - \nu} \Delta_{m',n'} \right\} \Delta_{m,n} \sum_{\nu} \frac{i}{\omega - \nu} \Delta_{m',n'} \sum_{\nu} \frac{i}{\omega - \nu} \Delta_{m,n} \sum_{\nu} \frac{i}{\omega - \nu} \Delta_{m',n'}
\]

(6-27)
To do the \( \omega \) integration in (6-27), the analytic properties of \( \Delta^0(\omega) \) and \( \Delta^1(\omega) \) as functions of the complex variable \( \omega \) are needed. These have already been given in Appendix 3. For both \( \Delta^0 \) and \( \Delta^1 \) there is a cut just below the real axis, extending from \( \varphi^2 \) to \( +\infty \) with an extra pole somewhere along this cut. These singularities are shown in figure 6-6. The two poles of \( G^0(\omega; \omega-\xi) \) are also represented. If the contour is completed above, only one contribution occurs, namely from the simple pole \( \omega = \varphi^2 + \xi + i\eta \). Hence (6-27) becomes

\[
\begin{align*}
\Theta_1 &= -\frac{1}{\sqrt{m \cdot m'}} \sum_{m, m'} \delta_{p, m + \epsilon} \delta_{q, m', 0} \sum_{m''} \frac{1}{2\pi i} \int \frac{d\xi}{\varphi^2} C^0(m''; \epsilon) (-i) \xi m'' \Delta^0 \left( m'' + \xi + i\eta \right) \Delta^1 \left( m'' + \xi + i\eta \right) \\
&= -\frac{1}{\sqrt{m \cdot m'}} \sum_{m, m'} \delta_{p, m + \epsilon} \delta_{q, m', 0} \sum_{m''} \frac{1}{2\pi i} \int \frac{d\xi}{\varphi^2} C^0(m''; \epsilon) \Delta^0 \left( m'' + \xi + i\eta \right) \Delta^1 \left( m'' + \xi + i\eta \right) . \tag{6-28}
\end{align*}
\]

Because of translational invariance, \( m + \epsilon = m'' + m'' \) in \( \Delta^0 \) and similarly for the conjugate equation. Alternatively, this can be concluded from the iterated solution of the equation for the Bethe-Goldstone amplitude. Hence in (6-28) \( m'' = \varphi \), from which

**Figure 6-6**

\( \omega \)-plane

\[ \omega^2 + \xi + i\eta \]

Singularities of \( \Delta^0 \) and \( \Delta^1 \)

Singularities of the integrand in (6-27).
we conclude that

\[ \Theta_P = \frac{i\lambda}{\sqrt{2}} \sum_{m,m'} \sum_{m,m'} \sum_{m,m'} \left( \Delta \right) \sum_{m,m'} \left( \frac{e+i\pi}{2} \right) \theta^{\text{on}} \left( \frac{e+i\pi}{2} \right). \]  

(6.21)

Finally, noting that \( \Delta \theta^{\text{on}} \theta^{\text{on}} = \theta^{\text{on}} \), equation (6-29) becomes

\[ \Theta_P = \frac{i\lambda}{\sqrt{2}} \sum_{m,m'} \sum_{m,m'} \left( \Delta \right) \left( \frac{e+i\pi}{2} \right)^2. \]  

(6.30)

Introducing a frequency dependent enhancement factor \( \xi(q) \) defined as

\[ \xi(q) = \left( \sum_{m,m'} \left( \frac{e+i\pi}{2} \right)^2 \right). \]  

(6.31)

we get for the partial annihilation rate

\[ \Theta_P = \frac{i\lambda}{\sqrt{2}} \sum_{m,m'} \sum_{m,m'} \left( \Delta \right) \xi(q) \left( \frac{e+i\pi}{2} \right). \]  

(6.32)

It is clear now that if the enhancement factor were not frequency dependent, we would get formula (6-12). The correct expression however does involve a frequency dependent enhancement factor which is just the mathematical statement that for an electron above the sea there is an uncertainty in its energy which must be accounted for.

A very similar calculation in which the positron self energy is allowed in one line only of an arbitrary ladder graph leads to the expression

\[ \Theta_P = \frac{i\lambda}{\sqrt{2}} \sum_{m,m'} \sum_{m,m'} \left( \Delta \right) \left( \frac{e+i\pi}{2} \right)^2. \]  

(6.33)

If an enhancement factor \( \xi(q) \) defined by
is introduced in (6-33) (where \( \vec{p} \) is the total momentum of the annihilating pair and \( \vec{q} \) is the positron momentum), it becomes

\[
\xi(q, t; \xi) = \left( \sum_m \Lambda_m^{(6-33) \partial / \partial \vec{q}} \right)^2
\]

(6-39)

Again the frequency dependence of the enhancement factor is apparent. The amplitude \( \frac{\partial}{\partial \vec{q}} \left( \epsilon + \vec{q} - \vec{p} \right) \) is the wave function for an electron and a positron inside a metal, which are asymptotically in plane wave states \( | \vec{p}, \vec{q}, \epsilon \rangle \) and \( | \vec{q}, \vec{p}, \epsilon \rangle \), respectively.

Next we ask whether the polarization term (i.e., diagram 5-1a) is enhanced in a similar fashion? The answer is yes. Consider the set of all ladder graphs with self energies neglected but with the dynamic potential \( \mathcal{U}(z, z') \) included in each step; that is, write

\[
\xi_p(\alpha', \beta') = \xi_{p}(\alpha, \beta) \cdot \xi_{p}(\alpha', \beta') - i \int d_3 \xi_{3} d_3 \xi_{3}' \xi_{p}(\alpha, \beta) \xi_{p}(\alpha', \beta') \mathcal{U}(\xi_{3}, \xi_{3}') \xi_{p}(\xi_{3}', \xi_{3})
\]

(6-36)

The \( n \)th order term in the iterated solution of (6-36) can be written symbolically as

\[
(\xi^{(n)}) \left( \xi_{p} \xi_{p} \cdot \xi_{p} \xi_{p} \cdots \xi_{p} \cdot \xi_{p} \right).
\]

(6-37)

In this expression, keeping only one dynamic effective potential function \( \mathcal{U}(z, z') \) (the others being approximated by their static limit) leads to \( n \) terms which are easily recognized as the \( n \) \( n \)th order terms in the expansion of

\[
-i \int \xi_{p}(\alpha, \beta, \gamma) \mathcal{U}(\gamma, \delta) \xi_{p}(\delta, \gamma) d_\gamma d_\delta,
\]

(6-38a)
with
\[ \mathcal{C}_p(\pi', \eta') = \mathcal{G}_p(\pi', \eta') + \int d^3 \xi \, \mathcal{G}_{\pi}(\pi', \eta') \mathcal{G}_{p}(\eta', \eta') \mathcal{C}_p(\xi'; \eta'). \] (6-38)

Note that expression (6-38) does not include the zeroth order term in (6-36), but this is precisely what we want. Equations (6-38) then represent the sum of all ladder graphs with the dynamic potential included in one and only one step. The contribution from (6-38) to the total annihilation rate is

\[ \left( \frac{\alpha^n}{\sqrt{3}} \right) \mathcal{I} \int d^3 \xi \, d^3 \eta \, e^{-i \mathcal{G}(\pi', \eta') \xi} \mathcal{C}_p(\pi'; \eta') \mathcal{C}_p(\xi'; \eta'). \] (6-39)

To evaluate (6-39), \( \mathcal{C}_p(\pi'; \eta') \) and \( \mathcal{C}_p(\pi'; \eta') \) are required for the general case \( \frac{1}{2} \neq \frac{1}{3} \), in contrast with the situation of Appendix 3 where \( \mathcal{C}_p \) was required for only \( \frac{1}{2} = \frac{1}{3} \). However this complication does not really present any difficulty. We need only realize that for \( \frac{1}{x} = \frac{1}{y} \), but \( \frac{1}{x} + \frac{1}{y} \), \( \mathcal{C}_p(\pi'; \eta') \) can be written as

\[ \mathcal{C}_p(\pi'; \eta') = \int d^3 \xi \, d^3 \eta \, e^{-i \mathcal{G}_{\pi}(\pi', \eta') \xi} \mathcal{C}_p(\xi'; \eta') \mathcal{C}_p(\xi'; \eta'), \] (6-40)

while for \( \frac{1}{x} + \frac{1}{y} \), but \( \frac{1}{x} = \frac{1}{y} \), it can be written as

\[ \mathcal{C}_p(\pi'; \eta') = \int d^3 \xi \, d^3 \eta \, e^{-i \mathcal{G}(\pi', \eta') \xi} \mathcal{C}_p(\eta'; \eta') \mathcal{C}_p(\eta'; \eta') \mathcal{D}^{(\pi'; \eta')} \mathcal{D}^{(\eta'; \eta')} \] (6-41)

where \( \mathcal{D}^{(\pi'; \eta')} \) is required only for \( \frac{1}{x} = \frac{1}{y} \), \( \frac{1}{z} = \frac{1}{y} \), and when Fourier transformed it satisfies the now standard equation (6-22). A similar situation holds for the conjugate function \( \mathcal{D}^{(\pi', \eta')} \).

Introducing (6-40) and (6-41) into (6-39), Fourier transforming, and simplifying gives
\[ \Theta_\text{f} = \frac{(2\pi)^3}{V^2} \int \frac{d\omega d\varepsilon d\nu}{(2\pi)^3} \left[ \sum_{\text{m, m', } \text{odd, even}} \int \frac{d\kappa}{(2\pi)^2} \right] \rho_\text{f}^{(\epsilon_\text{f}')} \left( \begin{array}{c} \text{even} \\ \text{odd} \end{array} \right) \delta_\text{f}^{(\epsilon_\text{f}')} (\kappa) \mathbf{c}_\text{f}^{(\epsilon_\text{f}')} (\kappa; \varepsilon_\text{f}'; \nu + \omega) \mathbf{c}_\text{f}^{(\epsilon_\text{f}')} (\kappa; \varepsilon_\text{f}'; \nu - \omega) \right] \]

But observe that \( m_1 + m_2 = \frac{q}{2}, \ m_1 + m_2 = \frac{p}{2}, \) with \( p > q \) allows us to drop the second term in both (6-22) and (6-23) and so replace them by (6-25) and (6-26). Hence as functions of \( \theta' \) the amplitudes \( \Delta^0 \) and \( \Delta^0_+ \) have all their singularities in the lower half plane as shown in figure 6-6. A knowledge of these singularities can be used to work out

\[ \left( \frac{\Delta_0}{2\pi} \right) \mathbf{c}_\text{f}^{(\epsilon_\text{f}')} (\kappa; \varepsilon_\text{f}'; \nu - \omega) \mathbf{c}_\text{f}^{(\epsilon_\text{f}')} (\kappa; \varepsilon_\text{f}'; \nu + \omega) \mathbf{c}_\text{f}^{(\epsilon_\text{f}')} (\kappa; \varepsilon_\text{f}'; \nu - \omega) \mathbf{c}_\text{f}^{(\epsilon_\text{f}')} (\kappa; \varepsilon_\text{f}'; \nu + \omega) \]

where the term involving two positron theta functions of the form \( \delta(-k) \) was discarded as usual. Thus \( \Theta_\text{f} \) becomes

\[ \Theta_\text{f} = \frac{2\lambda^3}{V^2} \int \frac{d\omega d\varepsilon d\nu}{(2\pi)^3} \left[ \sum_{\text{m, m', } \text{odd, even}} \int \frac{d\kappa}{(2\pi)^2} \right] \rho_\text{f}^{(\epsilon_\text{f}')} \left( \begin{array}{c} \text{even} \\ \text{odd} \end{array} \right) \delta_\text{f}^{(\epsilon_\text{f}')} (\kappa) \mathbf{c}_\text{f}^{(\epsilon_\text{f}')} (\kappa; \varepsilon_\text{f}'; \nu + \omega) \mathbf{c}_\text{f}^{(\epsilon_\text{f}')} (\kappa; \varepsilon_\text{f}'; \nu - \omega) \right] \]

The translational invariance of the theory guarantees that

\[ \Delta^0_+ (\kappa, \varepsilon_\text{f}; \nu) = 0 \] unless \( m_1' + m_2' = m_1 + m_2 \). This implies that \( \kappa' = \frac{p}{2} \) in (6-44), giving
\[ \Theta_f = \frac{2i}{\sqrt{d_f}} \left( \frac{\delta}{\delta \nu_f} \Delta^{(0)}(q; \epsilon) \right) \left( \frac{\delta}{\delta \nu_f} \Delta^{(0)}(q; \epsilon) \right) \left( \frac{\delta}{\delta \nu_f} \Delta^{(0)}(q; \epsilon) \right) \]  

(6-45)

with

\[ \Delta^{(0)}(q; \epsilon) = \frac{\delta(q - q')}{(p - \epsilon - i\eta)^2} \left( \frac{\delta}{\delta \nu_f} \right) U(q; \nu) G^0(q + \nu; \nu + i\eta) \frac{1}{i^2 q - i\nu - \eta} \]  

(6-46)

Summary.

The sum of all ladder graphs with electron self energies kept to first order in one and only one of the electron lines in each ladder graph, while the positron lines are all taken to be free propagators, is shown in figure 6-7b. Its contribution to \( \Theta_f \) can be written in the form (6-30). Similarly, for positron self energies, the contribution to \( \Theta_f \) from the sum of all the graphs of figure 6-7c is given by (6-33). If however the self energy effects are neglected but the dynamic potential is kept in one and only one of the steps in each ladder graphs as shown in figure 6-7a, then we are led to a contribution to \( \Theta_f \) of the form (6-45).

The task now is to show that the sum of these three contributions to \( \Theta_f \) (denoted respectively by \( \Theta_f^a \), \( \Theta_f^b \), and \( \Theta_f^c \)) is almost zero, not because they are individually small but because \( \Theta_f^a \) is negative and in absolute value approximately equal to the sum of \( \Theta_f^b \) and \( \Theta_f^c \). To begin, consider the electron self energy case. Since for \( p^0 q_f \),

\[ G^0_c(q; \epsilon) = \frac{\delta(p - q_f)}{(p - \epsilon - i\eta)^2} \left( \frac{\delta}{\delta \nu_f} \right) U(q; \nu) G^0(q + \nu; \nu + i\eta) \]  

(6-47)

equation (6-30) gives that
The sum (a) of all ladder graphs with dynamic potential included in one and only one step in each order of perturbation theory. The sum (b) of all ladder graphs with electron self energies included in one and only one of the electron lines in each order (all positron propagators are free propagators). The sum (c) is a similar sum including positron self energies in one and only one line in each order.

\[ \Theta_{\text{p}}(\xi) = \frac{U_{\text{p}}^2}{V^2} \sum \left[ \frac{d\sigma}{d\Omega} \right] \frac{d\xi}{2\pi} \frac{G_{\text{p}}(\xi, \eta)}{\xi^2 - \eta^2} \left( \prod \Delta_{\text{m}, \Delta_{\text{m}}, \xi - \eta} \right) \]  \hspace{1cm} (6.48)

The $\xi$ integration in (6.48) can be done simply by closing the contour above. Since the amplitude $R^0$ is analytic in the upper half plane we get
\[ \Theta_{\mathbf{q}^+}^7 = \frac{i\lambda}{\sqrt{2}} \sum_{\mathbf{m}, \mathbf{n}} \int \frac{d^4 q}{(2\pi)^4} \frac{U(q, \mathbf{m}) \Theta(E_{\mathbf{m}} + \mathbf{q} - \mathbf{q}^+)}{(p^2 - m^2 - n^2 + i\eta)^2} \left( \sum_{\mathbf{m}, \mathbf{n}} p_{\mathbf{m}, \mathbf{n}} \right)^2. \]  

(6.49)

If \( \Theta_{\mathbf{q}^+}^{7c} \) and \( \Theta_{\mathbf{q}^+}^{7a} \) are reduced by similar methods, the sum of \( \Theta_{\mathbf{q}^+}^{7b} \) and \( \Theta_{\mathbf{q}^+}^{7c} \) can be written as

\[ \Theta_{\mathbf{q}^+}^{7b} + \Theta_{\mathbf{q}^+}^{7c} = \frac{i\lambda}{\sqrt{2}} \sum_{\mathbf{m}, \mathbf{n}} \int \frac{d^4 q}{(2\pi)^4} \frac{U(q, \mathbf{m}) \Theta(E_{\mathbf{m}} + \mathbf{q} - \mathbf{q}^+)}{(p^2 - m^2 - n^2 + i\eta)^2} \left( \sum_{\mathbf{m}, \mathbf{n}} p_{\mathbf{m}, \mathbf{n}} \right)^2. \]  

(6.50)

Suppose that in (6-50) the amplitudes \( \mathcal{N}_{\mathbf{m}, \mathbf{n}}(\mathbf{q}^+) \) are replaced by their lowest approximation \( S_{\mathbf{m}, \mathbf{n}} \). Then (6-50) reduces to the sum \( \Theta_{\mathbf{q}^+}^{1a} + \Theta_{\mathbf{q}^+}^{1b} + \Theta_{\mathbf{q}^+}^{1c} \), which is very nearly zero as was shown in the first part of this chapter. Next suppose these amplitudes are treated in the Born approximation, i.e. write \( \sum_{\mathbf{m}, \mathbf{n}} \mathcal{N}_{\mathbf{m}, \mathbf{n}}(\mathbf{q}^+) = 1 + \chi^{(0)}(\mathbf{q}^+) \)

where

\[ \chi^{(0)}(n + \mathbf{q} - \mathbf{q}^+) = \frac{i\lambda}{\sqrt{2}} \sum_{\mathbf{m}, \mathbf{n}} \frac{U(q, \mathbf{m}) \Theta(E_{\mathbf{m}} + \mathbf{q} - \mathbf{q}^+)}{(p^2 - m^2 - n^2 + i\eta)^2} \left( \sum_{\mathbf{m}, \mathbf{n}} p_{\mathbf{m}, \mathbf{n}} \right)^2. \]  

(6.51)

with a similar expression for \( \sum_{\mathbf{m}, \mathbf{n}} \mathcal{N}_{\mathbf{m}, \mathbf{n}}(\mathbf{q}^+) \). Besides the zeroth order contribution \( \Theta_{\mathbf{q}^+}^{(1a+1b+1c)} \), this leads to four first order contributions which can be grouped in pairs according to whether they involve the first order correction to \( \mathcal{N}_{\mathbf{m}, \mathbf{n}}(\mathbf{q}^+) \) or to \( \mathcal{N}_{\mathbf{m}, \mathbf{n}}(\mathbf{q}^+) \). Denoting the simplest of these pairs by
where the first term \( \Theta_{\Phi}^{(1)} \) comes from electron self energies while the second \( \Theta_{\Phi}^{(2)} \) comes from the polarization. (The second pair is very similar. It represents a contribution from positron self energies together with another from the polarization.) The integral (6-52) is quite complicated but can be reduced analytically to a triple integral and evaluated on a computer. For the numerical results see Appendix 6. There we find, as expected, that \( \Theta_{\Phi}^{(1)} \) is negative and very nearly equal in absolute value to \( \Theta_{\Phi}^{(2)} \). Assuming that similar results hold for the second pair (this is a reasonable assumption), we get that \( \Theta_{\Phi}^{(1)} + \Theta_{\Phi}^{(2)} + \Theta_{\Phi}^{(3)} = 0 \) in the Born approximation.

It should be clear now that this cancellation can be expected to occur even in the most general case. We can give quite a simple argument why this must be so. Begin by replacing \( \Delta_{0,m,\pm m; \pm \mp, \mp} \) by \( \Delta_{0,m, \pm m; \pm \mp, 0} \) in (6-50). This leads to

\[
\Theta_{\Phi}^{(1)} + \Theta_{\Phi}^{(2)} + \Theta_{\Phi}^{(3)} = \frac{i}{2} \int \frac{d\omega}{2\pi} \omega \Theta(\omega^{-1} - q^{-1}) \left[ \frac{1}{(q^{-2} - 2\omega^{-1} - \omega - i\gamma)^2} \right]
\]

Now do the \( \omega \) integration in (6-53). Since the amplitude \( \Delta_{0} \) is analytic in the upper half plane, closing the contour above results in only two contributions, one from the plasmon pole which we neg-
The variation with energy $E$ of $F_{\text{f}}(E)$ and $6.5 \chi_{\text{f}}^{(4)}(E)$ for $\eta=4$ and $p=1.1 p_F$. The quantity $\bar{E}$ is dimensionless: $\bar{E} = 1$ corresponds to $E = 0$. The calculation was also done for $p=1.3 p_F$, $1.5 p_F$ and $1.7 p_F$. The curves for these values are very similar. An excellent check that the range of energy plotted is more than sufficient is that from the exact values for $\chi_{\text{f}}^{(4)}$, $\chi_{\text{f}}^{(1)}$ and $\chi_{\text{f}}^{(0)}(E)$ one finds that (for $\eta=4$, $p=1.1$, 1.3, 1.5, 1.7 $p_F$) $\chi_{\text{f}}^{(4)} = (\chi_{\text{f}}^{(1)})^2 \chi_{\text{f}}^{(5)}(E=15 p_F)$ and similarly $\chi_{\text{f}}^{(4)} = (\chi_{\text{f}}^{(1)})^2 \chi_{\text{f}}^{(5)}(E=95 p_F)$. This should also give us confidence that the energy dependence of the amplitudes appearing in (6-53) is not important.
lect and another from the cut. Thus

\[
\Theta_{\frac{1}{2}} \rho_{0}^{1} + Q_{1}^{\nu} + R_{\frac{1}{2}}^{\nu} = \frac{1}{V^2} \int \frac{d\omega}{2} \left( \frac{1}{b^2 + \omega} \right) \Theta_{\frac{1}{2}} \rho_{0}^{1} \rho_{b}^{1} \int \frac{d\omega}{2} \left( \frac{1}{b^2 + \omega} \right)
\]

where for \( \nu < 0 \)

\[
\Theta_{\frac{1}{2}} \rho_{0}^{1} = \frac{2 \pi}{b^2} \sum_{m} \Theta_{\frac{1}{2}} \rho_{b}^{1} \Theta_{\frac{1}{2}} \rho_{b}^{1} S(x + \nu (b^2 - \omega))
\]

Next write \( E = \alpha + (\nu \theta^2) \), and notice that \( E \) is certainly bounded to the range \( (b^2 - \nu \rho^2) \). Also, because of the energy denominators in (6-54), it is clear that the most important part of this range is \( E \approx \rho^2 \). If we define \( F_{\frac{1}{2}}(E) = \left( \sum_{m} \Theta_{\frac{1}{2}} \rho_{b}^{1} \rho_{b}^{1} \right)^2 \) and evaluate it numerically, we find that \( F_{\frac{1}{2}}(E) \) is a slowly varying function of energy in the range \( E \approx \rho^2 \) (See figure 6-8). Thus we can take it out of the integral (6-54) giving \( \Theta_{\frac{1}{2}} \rho_{0}^{1} + Q_{1}^{\nu} + R_{\frac{1}{2}}^{\nu} \approx
\]

\( \Theta_{\frac{1}{2}} \rho_{0}^{1} + Q_{1}^{\nu} + R_{\frac{1}{2}}^{\nu} \) \( E_{\omega} \) \( \approx \Omega \). This is what we set out to show.

We can in fact make a slightly better calculation. We know from direct evaluation of (6-52) that \( \Theta_{\frac{1}{2}} \rho_{0}^{1} \) and \( \Theta_{\frac{1}{2}} \rho_{0}^{1} \) are almost the same in absolute value. It appears then that replacing one of the two denominators \( (b^2 - \nu \rho^2) \) by \( (\nu^2 - \omega - \eta) \) does not significantly change its value. Assuming that changing both denominators makes little difference as well, we can conclude that

\[
\frac{1}{V^2} \int \frac{d\omega}{2} \left( \frac{1}{b^2 - \nu \rho^2 - \omega - \eta} \right) \Theta_{\frac{1}{2}} \rho_{0}^{1} \rho_{b}^{1} \int \frac{d\omega}{2} \left( \frac{1}{b^2 - \nu \rho^2 - \omega - \eta} \right) \rho_{b}^{1} \rho_{b}^{1} \Theta_{\frac{1}{2}} \rho_{b}^{1} \Theta_{\frac{1}{2}} \rho_{b}^{1} S(x + \nu (b^2 - \omega)) \approx 0
\]

*(For the details of this numerical evaluation see section VI in K-II. Our equation is almost identical.*)
But doing the \( \pi \) integration in (6-55) and dropping the plasmon part gives (6-54) with \( f_\pi(E) = \left( \frac{\hbar}{m} \right) \frac{\delta(E)}{\delta \pi^0, \pi^+} \) replaced by

\[ \chi^{(l)}(E = \sqrt{t^2 + (\pi^0 - 1)^2}) \] . Finally the numerical evaluation of \( \chi^{(l)}(E) \) shows that \( f_\pi(E) \geq (const.) \chi^{(l)}(E) \) (see figure 6-8). Thus we again get that \( \mathcal{R}_a^{\pi} + \mathcal{R}_b^{\pi} + \mathcal{R}_c^{\pi} \equiv 0 \).

Final note.

The results of Chapters 3, 4, 5, and 6 can be summarized by a single statement: Positron annihilation in a fully interacting electron gas is described adequately by Kahana's enhancement factors. They can be considered to include self energy effects and no corrections are necessary for hole-particle interactions.
Chapter 7

EFFECT OF THE LATTICE ON POSITRON ANNIHILATION IN SODIUM

Introduction.

The presence of the lattice can modify the results of positron annihilation in a valence electron gas in two major ways. First, the valence electrons as well as the positron are not in plane wave states, even when their coulomb interactions are neglected. Instead they are in Bloch states. This modification has already been discussed in Chapter 1; briefly, it can be accounted for by changing the basic elements of the perturbation series from

\[ C_{e}^n(x',x) = \sum_{l} \int \frac{d^{3}q}{(2\pi)^{3}} \phi_{e}(x' - q) \phi_{e}(x + q) \]

and

\[ C_{p}^n(x',x) = \sum_{l} \int \frac{d^{3}q}{(2\pi)^{3}} \phi_{p}(x' - q) \phi_{p}(x + q) \]

respectively. The notation in 7.1b is as given in 1-44 and 1-46. The second modification is the existence of the core electrons and hence the possibility of core annihilation. Both of these effects will be discussed in connection with sodium. It is well known that sodium is a "good" metal in the sense that the valence
electrons are nearly free. For the occupied part of the valence band up to the Fermi level, the constant energy surfaces are very nearly spherical, the $E$ by $k$ relationship is almost parabolic, and the Bloch states do not differ very much from plane waves. It is precisely because of these reasons that we are interested in sodium. The hope is that for sodium the presence of the lattice will have little effect other than introducing core annihilation, and so serve as a test case for the theory of positron annihilation in an interacting electron gas as developed in the previous chapters.

Calculations of the effect of the lattice on the angular correlation problem as well as on the total annihilation rates have been carried out in the past by Berko and Plaskett\(^{(10)}\) for copper and aluminium, and by Daniel\(^{(9)}\) for copper. Their calculations are straightforward and we will use a similar approach. From the beginning all interactions except the presence of the crystal field are neglected. In a first section the geometrical properties of the sodium lattice are discussed. Next, Callaway's calculation\(^{(8)}\) of the valence electron Bloch states is considered. He uses a cellular method in the spherical approximation (Wigner-Seitz approximation) which yields wave functions in one basic atomic polyhedron. These functions must then be continued periodically throughout the entire crystal. From the Bloch states the angular correlation curve is computed. It deviates only slightly from an inverted parabola in the region $(0, \theta_c)$ with very narrow but long "tails" beyond the cut-off angle $\theta_c$. These tails can account for only a small part of the broad experimental tails. Next the positron Bloch state is determined, and its effect on the angular correlation curve (excluded volume effect) is found
to be even smaller. From a knowledge of the positron wave function, core annihilation is estimated on a rigid ion model. This yields a value of 1.02 $\theta$ for the contribution of core electrons to the total annihilation rate, and introduces long and broad "tails" in the photon angular distribution. Finally, the problem of an enhancement factor for core annihilation is mentioned briefly.

Geometry of the sodium lattice.

The crystal structure of metallic sodium is body-centered cubic. A set of primitive translation vectors appropriate to this spatial array is $\mathbf{v}_1 = \frac{1}{2}a(-\xi_1 - \xi_2 + \xi_3)$, $\mathbf{v}_2 = \frac{1}{2}a(\xi_1 + \xi_2 + \xi_3)$, and $\mathbf{v}_3 = \frac{1}{2}a(-\xi_1 + \xi_2 - \xi_3)$, where $\xi_1, \xi_2, \xi_3$ is an orthonormal set of vectors along the cube edges as shown in figure 7-1a, and $a$ is the edge length. Each primitive cell has a volume $V = \mathbf{v}_1 \cdot \mathbf{v}_2 \times \mathbf{v}_3 = \frac{1}{2} a^2$ and contains one atom. Sodium has only one valence electron; this gives a volume of $\frac{1}{4} a^2$ per valence electron. The corresponding $\sigma$ parameter is determined by writing $2\pi^2 \frac{1}{3} a^2$. At zero degrees Kelvin, $\sigma = 2.94$ and $a = 0.36$ Bohr units. A slightly larger $\sigma$ would be more appropriate for the positron annihilation

Figure 7-1

![Diagram](image-url)
problem. However, since Callaway's work on the Bloch states of
the valence electrons is for 0\degree K, we will use $a = 194$. By def-
inition, the reciprocal lattice has the basis $b_1 = \frac{a_1}{\alpha}(a_1 - a_2)$,
$b_2 = \frac{a_1}{\alpha}(a_1 - a_2)$, and $b_3 = \frac{a_1}{\alpha}(a_1 - a_2)$. The various inverse
lattice sites are at $\gamma_\beta = \gamma_\alpha \gamma_\delta$ with $\gamma_\alpha$ integral (or $\gamma_\alpha = \gamma_\delta$,
$\gamma_\delta$ integral and $m_1 + m_2 + m_3$ even). This is a face-centered cubic
lattice as shown in figure 7-1b. Each reciprocal lattice site
has twelve nearest neighbours at a distance of $\frac{\alpha}{\gamma}$ inverse Bohr
units. Table 7-1 goes up to the eleventh nearest neighbours,
giving the distance and the number of each kind. These parameters

<table>
<thead>
<tr>
<th>1' th nearest neighbour</th>
<th>number of such neighbours</th>
<th>distance in inverse Bohr units</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>12</td>
<td>(4 / ) $\sqrt{3} = 1.1104$</td>
</tr>
<tr>
<td>2</td>
<td>6</td>
<td>(&quot; &quot; ) $\sqrt{3} = 1.5704$</td>
</tr>
<tr>
<td>3</td>
<td>24</td>
<td>(&quot; &quot; ) $\sqrt{3} = 1.9233$</td>
</tr>
<tr>
<td>4</td>
<td>12</td>
<td>(&quot; &quot; ) $\sqrt{3} = 2.2009$</td>
</tr>
<tr>
<td>5</td>
<td>24</td>
<td>(&quot; &quot; ) $\sqrt{3} = 2.4330$</td>
</tr>
<tr>
<td>6</td>
<td>8</td>
<td>(&quot; &quot; ) $\sqrt{3} = 2.7200$</td>
</tr>
<tr>
<td>7</td>
<td>48</td>
<td>(&quot; &quot; ) $\sqrt{3} = 2.9379$</td>
</tr>
<tr>
<td>8</td>
<td>6</td>
<td>(&quot; &quot; ) $\sqrt{3} = 3.1408$</td>
</tr>
<tr>
<td>9</td>
<td>12</td>
<td>(&quot; &quot; ) $\sqrt{3} = 3.3313$</td>
</tr>
<tr>
<td>10</td>
<td>24</td>
<td>(&quot; &quot; ) $\sqrt{3} = 3.5115$</td>
</tr>
<tr>
<td>11</td>
<td>24</td>
<td>(&quot; &quot; ) $\sqrt{3} = 3.6829$</td>
</tr>
</tbody>
</table>

The distance from the origin of the first eleven lattice
vectors $\gamma_\alpha$ and the number of each kind.

are needed when one wants to continue periodically throughout the
entire crystal a Wigner-Seitz wave function known only in a
single atomic polyhedron. This completes the discussion of the
relevant parameters of the sodium lattice.
Electron Bloch states

Neglect all coulomb interactions and concentrate on the effect of the crystal field on the valence electrons. In this approximation the partial annihilation rate $R_{f}$ is simply given by

$$R_{f} = \frac{e^{2}}{\hbar} \int \frac{d^{3}q}{2\hbar} \frac{d^{3}q}{2\hbar} \frac{d^{3}q}{2\hbar} \frac{d^{3}q}{2\hbar} a_{f}^{-} \gamma^{(\lambda \cdot \mathbf{q})} C_{\alpha}^{\ast}(\mathbf{q}, \gamma^{+}) C_{\beta}^{\ast}(\mathbf{q}, \gamma^{+}),$$

(7-2)

with $C_{\alpha}^{\ast}(\mathbf{q}, \gamma^{+})$ defined by (7-1b). The choice of the crystal potential $\Phi(\mathbf{r})$ seen by a valence electron requires some care. If we were using the full perturbation series for the electron-positron correlation function, the appropriate crystal field $\Phi(\mathbf{r})$ would have to include only the potential coming from the ions, since the coulomb interactions would be accounted for by the perturbation series itself. However, this is not the potential that is normally used in energy band calculations. There the crystal field is chosen to include as much of the valence electron coulomb and exchange interactions as possible. In fact the valence electrons are conceived of as independent particles, each of which is moving in an average self consistent field of the Hartree-Fock type, coming from all other electrons as well as from the ions. The potential used in C-I is of this latter type. However provided we do not go beyond the simple approximation (7-2), we are clearly at liberty to include some of the coulomb interactions in the crystal potential $\Phi(\mathbf{r})$, and thus using the Bloch states as given in C-I is not inconsistent.

For the details of the crystal potential and the calculation of the valence electron Bloch states refer to C-I. The results are as follows. The valence electrons occupy only half of the
first Brillouin zone so that no band index is needed to specify the Bloch states. If we write these as \( \psi_k(x) = \frac{1}{\sqrt{V}} \sum_{\alpha, \beta} \hat{a}_{\alpha, \beta}^+ \psi_{\alpha, \beta}(x) \)

then \( \psi_k(x) \) in one atomic polyhedron (approximated by a sphere of equal volume according to the method of Wigner and Seitz) is given by

\[
\psi_k(x) = \psi_0(x) + \frac{i k \cdot x}{\hbar} \chi_0(x) + \frac{(k \cdot x)^2}{\hbar^2} \frac{3}{2} \psi_2(x) + k^2 (\phi_0(x) - \frac{1}{\hbar} \chi_0(x)),
\]

(7-1)

where \( \psi \) stands for \( \| \psi \| \). The radial functions \( \psi_0, \psi_1, \psi_2 \) and \( \phi_0 \) are tabulated in C-I. The energy corresponding to the state \( \psi_k(x) \) is not a parabolic function of \( k \), but the constant energy surfaces are still spherical so that the Fermi momentum remains correctly given by \( k_F = \frac{\pi q}{\sqrt{2}} \) (in inverse Bohr units). To extend \( \psi_k(x) \) to the entire crystal we expand it in Fourier series

\[
\sum_{\chi_0} \chi_0(x) a_{x, y} \chi_0(x).
\]

The Fourier coefficients \( a_{x, y} \) are given by

\[
\psi_k(x) = \psi_0(x) + \frac{i k \cdot x}{\hbar} \chi_0(x) + \frac{(k \cdot x)^2}{\hbar^2} \frac{3}{2} \psi_2(x) + k^2 (\phi_0(x) - \frac{1}{\hbar} \chi_0(x)),
\]

(7-1)

To begin, neglect the \( k \) dependence of \( \psi_k(x) \), i.e. set \( \psi_k = \psi_0 \).

In this approximation \( \psi_k(x) = \psi_0(x, \chi_0) \) where

\[
\psi_0(x, \chi_0) = \frac{1}{\sqrt{V}} \sum_{\alpha, \beta} \left( \psi_{\alpha, \beta}(x) - \psi_{\alpha, \beta}(x) \right) + \psi_{\alpha, \beta}(x) \frac{1}{\hbar} \chi_0(x).
\]

(7-5)

In the first term on the right hand side of (7-5) it is possible to replace, with very little error, the atomic polyhedron by the Wigner-Seitz sphere since around \( n = \chi_0 \) the integrand should almost vanish. Note that \( \psi_0(x, \chi_0) \) can depend only on \( \| \chi_0 \| \) and not on its direction. From the table of \( \psi_0(x) \) (properly normalized) given in C-I, (7-5) can be evaluated numerically. The Fourier coefficients for the eleven values of \( \| \chi_0 \| \) listed in Table 7-1 and
The $u_0(x_n)$'s are the Fourier coefficients in the expansion of the electron Bloch state $u_0(x)$. The $v_0(x_n)$'s are similar coefficients for the lowest energy positron Bloch state.

for $x_{n\alpha}$ are presented in Table 7-2. As a check on this expansion, note that $\sum |u_0(x_n)|^2 = .998$. If for the moment the positron Bloch state is neglected, then $\Theta_\Phi$ is

$$\Theta_\Phi = \frac{1}{V} \sum_{\mathbf{k}_f, |\mathbf{k}| < |\mathbf{k}_f|} \left| \frac{1}{V} \int \frac{d^3p}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{r}} u_0(x) \frac{d^3q}{(2\pi)^3} \right|^2$$

$$= \frac{1}{V} \sum_{\mathbf{k}_f, |\mathbf{k}| < |\mathbf{k}_f|} \sum_{x_m} |u_0(x_n)|^2 \delta(x, x + |\mathbf{q}|, y_m). \tag{7-4}$$

This formula is very similar to formula (2-5) of the Sommerfeld theory and can be visualized geometrically as follows. About

| $u_0(x_n)$ | $|u_0(x_n)|^2$ | # of coeff. | $v_0(x_n)$ | $|v_0(x_n)|^2$ |
|-----------|-------------|-------------|-----------|-------------|
| .96390    | .92910      | 1           | .98620    | .97270      |
| -.04397   | .00193      | 12          | -.04394   | .00193      |
| -.03759   | .00141      | 6           | -.01463   | .00021      |
| -.02874   | .00083      | 24          | -.00374   | .00001      |
| -.02088   | .00044      | 12          | -.00059   | -           |
| -.01493   | .00022      | 24          | -.00016   | -           |
| -.01078   | .00012      | 8           | -.00036   | -           |
| -.00799   | .00006      | 48          | -.00047   | -           |
| -.00611   | .00004      | 6           | -.00039   | -           |
| -.00478   | .00002      | 12          | -.00019   | -           |
| -.00379   | .00001      | 24          | .00003    | -           |
| -.00299   | .00001      | 24          | .00021    | -           |
each inverse lattice site $\chi_n$ there is a sphere of radius $k_f$ occupied with probability $|u_0(\chi_n)|^2$. The remainder of momentum space is unoccupied. Now when $Q^2_k$ is summed over $q_x$ and $q_y$ for $q_z$ fixed in some direction $\hat{n}$, the plane $q_{z'}=q_z$ will in general cut more than one of the spheres $|q_{z'}-\chi_n|=k_f$. The contribution to $Q^2_{k_z}$ is just proportional to the area of the circles of intersection weighted by the appropriate occupational probability $|u_0(\chi_n)|^2$. If for example the direction of $\hat{n}$ is chosen along $\chi_z=\hat{\alpha}$, the plane $q_z=\hat{\alpha}$ will

Figure 7-2

Effect of electron Bloch states on the angular correlation curve, in lowest order perturbation theory.
cut through the set of spheres centered in the plane $\mathbf{r}^2 = \frac{2\pi}{\theta}$ if $\theta$ is $\leq \frac{2\pi}{\theta}$. As $\theta$ increases beyond .298 it will start to cut through the additional set of spheres centered in the plane $\mathbf{r}'^2 = \frac{2\pi}{\theta}$, etc. The angular correlation curve in this example is shown in figure 7-2. Note the discontinuity in slope at $\theta = \theta_c$ (i.e. $\theta = \frac{\pi}{\theta_c}$). It is clear that the crystal field has very little effect on $\theta_c$. The broad experimental tails certainly cannot be explained on this basis. Finally, if the approximation $\mathbf{u}_n \approx \mathbf{u}_g$ is lifted, the calculation becomes much more complex but a preliminary estimate showed that no significant change in the angular correlation curve results.

**Positron Bloch state.**

To determine the positron Bloch state a Wigner-Seitz method is quite appropriate. Following previous authors, in the basic atomic polyhedron the self-consistent crystal potential seen by the positron is taken to be the sum of the field of the ion core* centered in this cell plus the field coming from the negative charge of a valence electron smeared uniformly throughout the Wigner-Seitz sphere. Using this potential the positron wave function $\psi_0(\mathbf{r}) = \Phi^{(0)}(\mathbf{r})$ (spherically symmetric in the Wigner-Seitz sphere) was determined numerically for the lowest energy state, i.e. the bottom of the 1s band. The wave function $\Phi^{(0)}(\mathbf{r})$ is shown in figure 7-3 and corresponds to an energy of .13 Rydbergs. If $\Phi^{(0)}(\mathbf{r})$ is compared with a straight line of slope 1 (which would be the wave function if there were no potential) it is apparent that the

* (The core field was chosen to be the field of a rigid free sodium ion $\text{Na}^+$ computed from tables of the core electron wave functions as given by Hartree and Hartree.)
Figure 7-3

Normalized positron wave function $\tilde{\psi}_n(n)$ in the Wigner-Seitz sphere.

positron is excluded somewhat from the core. However, as will be shown in the next section, there is still a considerable amount of core annihilation; that is, overlap of the positron wave function with the core electron wave functions. Finally, it is interesting to note that at the bottom of the next band (2s) the energy eigenvalue is very much higher, approximately 2.22 Rydbergs.

Expanding the positron wave function in Fourier series

$$\sum_{\tilde{\kappa}} \psi_\kappa(n) \ e^{i\tilde{\kappa} \cdot \mathbf{r}}$$

gives the Fourier coefficients shown in Table 7-2. The sum $\sum_{\tilde{\kappa}} |\psi_\kappa(n)|^2$ is equal to .997 which is again a good check on this expansion. Comparing the $\psi_\kappa(n)$'s with the $\tilde{\psi}_n(n)$'s, one concludes that the positron Bloch state is less effective in producing tails that the electron Bloch states. If both electron and positron Bloch states are combined, a rough calculation showed that the tails of figure 7-2 should be increased by about 20%, which is still much too small to account for the large experimental tails.
Core annihilation.

From a knowledge of the positron Bloch state, core annihilation can be estimated on a rigid ion model. That is, assume that the tight binding approximation is valid for the core electrons. Then their wave function can be written as

\[ \psi_{\text{core}}(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{K}} \mathbf{K} \cdot \mathbf{R}_e \psi_{\text{core}}(\mathbf{r} - \mathbf{R}_e) \]  \hspace{1cm} (7-7)

with \( \psi_{\text{core}}(\mathbf{r}) = Y_{\ell m} P_\ell(r)/r \). The \( Y_{\ell m} \)'s are the spherical harmonics and the \( P_\ell \)'s are the radial part of the core electron wave functions as given by Hartree and Hartree for a free ion Na⁺. The crystal momentum \( \mathbf{K} \) is restricted to one zone and the occupied core bands are 1s, 2s, and 2p. Expression (7-7) leads to a partial annihilation rate

\[ \Delta_{\mathbf{K}} = \frac{1}{N} \sum_{\ell m} \Delta_{\mathbf{K}} \psi_{\ell m}^* \psi_{\ell m} = \frac{1}{N} \sum_{\ell m} \pi (\ell + 1) \int_0^{\infty} P_\ell(r) R_\ell(r) J_\ell^2(p) \, dp \]  \hspace{1cm} (7-8)

where \( J_\ell(p) \) is the \( \ell \) th spherical Bessel function. \( \star \) Introducing a factor of 2 for spin degeneracy and noting that \( 1/\lambda_0 \) is just the Sommerfeld density, (7-8) becomes

\[ \Delta_{\mathbf{K}} = (2 \pi + 1) \pi (\ell + 1) \int_0^{\infty} \frac{P_\ell(r) R_\ell(r) J_\ell^2(p)}{\lambda_0} \, dp \]  \hspace{1cm} (7-9a)

with

\[ \Delta_{\ell m} = \left| \int_0^{\infty} P_\ell(r) R_\ell(r) J_\ell^2(p) \, dp \right|^2. \]  \hspace{1cm} (7-9b)

\( \star \) (For the detailed manipulation see for example Berko and Plaskett.)
Further, the two quantities of interest, $\Theta$ and $\Theta_B$, can be written in terms of the $J_{\alpha\lambda}(\eta)$'s as

$$\Theta = \Theta_0 \sum_{\alpha \lambda} (2\lambda+1) \int_0^{\eta_0^2} \frac{d\eta}{\eta \Theta_0} \Theta_{\alpha\lambda}(\eta)$$  \hspace{1cm} (7-10)

and

$$\Theta_B = \Theta_0 \sum_{\alpha \lambda} (2\lambda+1) \int_0^{\eta_0^2} \frac{d\eta}{\eta \Theta_0} \Theta_{\alpha\lambda}(\eta).$$  \hspace{1cm} (7-11)

The results are as follows. The 1s electrons do not contribute significantly to core annihilation. The contribution to $\Theta$ from the 2s electrons is 0.232 $\Theta_0$ while for the 2p electrons it is $3 \times 0.262 \Theta_0$. Thus in this simple model core annihilation increases the total annihilation rate by 1.018 $\Theta_0$. The individual contributions from the 2s and the 2p core electrons to the angular correlation curve (in units of $\Theta_0$ per inverse Bohr unit) is shown in figure 7-4. The curve for the 2p electrons is to be multiplied by 3 to account for the degeneracy factor (2$\lambda+1$). A change of units in figure 7-4 is convenient for comparison with the inverted Sommerfeld parabola. In figure 7-5 we have plotted the total contribution from core annihilation to the angular correlation curve in units of $3\lambda $ $\Theta_0$, with momentum measured in units of $\eta_F$. It is clear that core annihilation introduces very long and broad tails.

If the enhancement factor for the valence electrons is taken to be of the order of 12 as given in K-II, and all of the tails are tentatively assigned to core annihilation, then to obtain agreement with experiment an enhancement factor of about 3 or 4 would have to be introduced for the core electrons. This would also be consistent with present results on the total annihilation
Figure 7-4

Contribution to $Q_{F}$ from the 2s and 2p core electrons. The curve for the 2p electrons is to be multiplied by 3 to account for the degeneracy factor $(2l+1)$. 
rate since it would add roughly a factor of $6 \times 10^9 \text{sec}^{-1}$, giving a final theoretical value of $3.2 \times 10^9 \text{sec}^{-1}$. However, this is not the only alternative open to us; an enhancement of tails in figure 7-2 by an amount of the same order as the central parabolic distribution could account for part of the experimental tails. A calculation of the enhancement factor for the core electrons would be useful.

**Figure 7-5**

Effect of core annihilation on the angular correlation curve.
A note on Beryllium.

There are some very interesting data available on the angular correlation curve for an oriented beryllium crystal. The two photon distribution shows marked differences in the various directions. To reproduce these curves is a quite difficult problem. One could begin by ignoring all enhancement effects and trying to evaluate $Q_0$ from formula (7-2). This requires a knowledge of both the electron and positron Bloch states. The positron Bloch state can be determined by using a Wigner-Seitz method. The results of such a calculation are shown graphically in figure 7-6. The positron is again not completely excluded from the core. Fourier expanding this function does not introduce significant higher momentum components, and a calculation of core annihilation gives tails adding about $0.2\alpha Q_0$ to the total rate. So again a considerable part of the experimental tails come from core annihilation.

The valence electron Bloch states in beryllium are not well known. There is of course the possibility of using orthogonalized plane waves. A single orthogonalized plane wave accounts partially for the presence of the cores but of course not for the lattice potential. If one makes a calculation of $\mathcal{G}_1$ on this basis, one finds negligible departures from an inverted parabola. We did not carry this calculation further; to go beyond would almost certainly require introducing the lattice potential.

The details of the calculations described above will not be given here because of the length of this thesis. However they have been kept and are available if someone should become interested in continuing with this problem.
Figure 7-6

Unnormalized positron wave function $f_n(r)$ in a Wigner-Seitz sphere.
Chapter 8

THERMALIZATION TIME OF A POSITRON IN A METAL

Introduction.

A basic assumption used in interpreting the experimental angular correlation data is that the positron is essentially thermalized on annihilation with one of the metallic electrons. This permits us to assign the lowest energy state to the positron. The validity of this assumption was demonstrated by G.E. Lee-Whiting. He assumed that a screened coulomb force acts between the positron and an electron of the metal. All further correlations, except the Pauli principle between the electrons, were neglected. In this model the ground state of the metal is just a filled Fermi sphere. Hence when the positron interacts with one of the valence electrons, it must transfer enough of its energy to the electron so as to knock it above the Fermi sea. Thus the positron loses its energy to the metal. The rate of energy loss in this approximation was calculated in LW-I using ordinary perturbation theory, with the result that for sodium the thermalization time is roughly of the order 100 times smaller than the annihilation lifetime. (The accuracy of this estimate is limited by the fact that the screening parameter which enters the specification of the electron-positron potential is to some extent arbitrary.) Clearly most of the positrons will be thermalized on annihilation and this is all that is of interest for the positron annihilation problem. It is therefore not our aim in this chapter to make a new calculation of the thermalization time. Instead we will simply give an alternate expression which will be shown to reduce to the result of LW-I in a certain
limit. However, our expression in its general form does not suffer from the inevitable arbitrariness in the choice of the screening parameter inherent in the approach of LW-I, and could be made the basis for a more accurate determination of the thermalization time should this become desirable.

The series for the positron propagator.

We begin by neglecting the lattice entirely, replacing it with a fixed background of positive charge neutralizing the system. Consider the positron propagator

$$G_{\phi}(\omega, \omega') = i \langle w | \phi(\omega) \phi^+(\omega') | w \rangle,$$

where $| w \rangle$ is the fully interacting Heisenberg ground state for the system of $N$ electrons representing the metal. Note that for $\omega \neq \omega'$, $G_{\phi}(\omega, \omega')$ vanishes. The zeroth approximation to $G_{\phi}(\omega, \omega')$ is of interest:

$$G_{\phi}^0(\omega, \omega') = \sum_k \frac{1}{\omega - k^2 - i\gamma},$$

or, by Fourier transforming (8-2),

$$G_{\phi}^0(\omega; \omega') = \frac{1}{\omega - \omega' - i\gamma}.$$

It must be stressed that the positron propagator (8-1) differs from that discussed in the previous chapters since it is an expectation value in the ground state of an $W$ electron system rather than a system of $N$ electrons plus a positron. However the formal perturbation solution for $G_{\phi}(\omega, \omega')$ in terms of Feynman graphs still holds; the only difference enters through the
The two diagrams which must be considered up to second order in the expansion of the positron propagator.

Keeping in mind that we have assumed the existence of a background of positive charge neutralizing the system, then besides \( G_i(\omega;\omega') \) the only Feynman graph in the expansion of \( G_i(\omega;\omega') \) which need be considered up to second order is diagram 8-1b. This diagram is immediately recognized as the second order part of the diagram shown in figure 8-2. It is natural then to drop 8-1b and replace it by 8-2.

First order positron exchange diagram with the coulomb potential replaced by the full dynamic effective potential. The first diagram on the right hand side is of course zero.

**The irreducible self energy operator.**

All improper self energy diagrams of the type 8-2 can be summed by writing down an integral equation for this sum. This equation is represented graphically in figure 8-3, and gives
where we have introduced the irreducible self energy operator \( \mathcal{M}(\xi; \omega) \) defined as

\[
\mathcal{M}(\xi; \omega) = \frac{i}{\sqrt{\xi}} \int \frac{d^3k}{(2\pi)^3} \, \text{u}(\xi; \omega) \, C_\gamma(\xi; \omega - \xi) \tag{8-6}
\]

Figure 8-3

Graphical representation of the integral equation for the sum of all improper self energy graphs of the type 8-2.

Note that the zeroth order positron propagator has also been included in the integral equation (8-5). We adopt \( \mathfrak{C}_\gamma(\xi; \omega') \) as our final approximation to the fully interacting propagator \( \mathfrak{G}_\gamma(\xi; \omega') \). Fourier transforming both equations (8-4) and (8-5) gives

\[
\mathcal{M}(\xi; \omega) = \frac{i}{\sqrt{\xi}} \int \frac{d^3k}{(2\pi)^3} \, \text{u}(\xi; \omega) \, C_\gamma(\xi; \omega - \xi) \tag{8-6}
\]

\[
\mathfrak{G}_\gamma(\xi; \omega) = \mathfrak{G}^*_\gamma(\xi; \omega) + \mathfrak{G}^*_\gamma(\xi; \omega) \, \mathcal{M}(\xi; \omega) \, \mathfrak{G}_\gamma(\xi; \omega), \tag{8-7}
\]

where \( \mathcal{M}(\xi; \omega) \) is the Fourier transform of the irreducible self energy operator. Substituting expression (8-3) into equation (8-6) yields
Analytic properties of $M(k;\omega)$ and $G_p(k;\omega)$.

The analytic properties of the integrand in (8-8) as a function of the complex variable $\xi$ are shown in figure 8-4, and consist of the singularities of $u(k;\xi)$ with an extra pole in the upper half plane coming from the propagator $G_p(k;\omega)$. To avoid this pole, close the contour below. Two distinct contributions arise, one from the cut and the other from the plasmon pole.

The result is

$$M(k;\omega) = \int \frac{dk}{2\pi} \left( \frac{1}{\xi^2 - \omega^2} \right) \frac{2\pi i}{k} \text{Im}[G(k;\xi)] \left( \frac{1}{(k^2 - \omega^2 + i\gamma)} \right)$$

where $\frac{1}{2\pi i} B_k$ is the residue or the potential at the plasmon pole and $\omega_p$ is the plasmon energy. The imaginary part of $G(k;\xi)$ for $\omega > 0$ is
As a function of the complex variable $\omega$, the irreducible self energy operator $M(k;\omega)$ has a cut extending from 0 to $+\infty$ just below the real axis (coming from the continuum), while the plasmon introduces a further cut in part of this range. Hence $M(k;\omega)$ is analytic in the upper half plane. The formal solution of equation (8-7) gives that the positron Green's function is related to $M(k;\omega)$ by

$$G_p(k;\omega) = \frac{1}{(\omega^2 - M(k;\omega))}. \quad (8-12)$$

Provided that no new pole is introduced because of the appearance of the irreducible self energy operator in a denominator, it is clear that $G_p(k;\omega)$ has the same singularities as $M(k;\omega)$. Assuming that no such pole can occur, (8-12) can readily be inverted to get $G_p(k;\gamma)$:

$$G_p(k;\gamma) = \int_0^{+\infty} \frac{d\omega}{2\pi} \frac{e^{-i\omega\gamma}}{\omega^2 - M(k;\omega)} \quad (8-13)$$

$$= \begin{cases} 0 & \text{for } \gamma < 0 \\ \int_0^{\infty} \frac{d\omega}{2\pi} \frac{e^{-i\omega\gamma}}{(\omega^2 - E(k;\gamma))^2 + \frac{1}{4} M(k;\gamma)} & \text{for } \gamma > 0 \end{cases} \quad (8-14)$$
where \( \frac{1}{2} \mathcal{I}(k, q) \) is the imaginary part of \( M(k, \omega) \) along the cut and \( \mathcal{R}(k, q) \) is its real part. For instance,

\[
\frac{1}{2} \mathcal{I}(k, q) = \frac{\pi}{V} \sum_{J=1}^{\infty} \delta(k - q) \delta\left(\frac{k^2 + q^2}{2} - \omega^2\right) \mathcal{S}
\]

The integral (8-14) is similar to the integral entering the theory of damping of quasi-particles (or quasi-holes) and there is no difficulty in evaluating it for \( \gamma \ll 1 \). Assuming that the perturbation theory is valid, then since \( \mathcal{R}(k, q) \sim O(\alpha) \) and \( \mathcal{I}(k, q) \sim O(\alpha^2) \) we can conclude that these are small as compared to 1. Thus the integrand is peaked about \( q = k^2 \mathcal{R}(k, q) \) \( \approx k^2 \); so replacing \( \mathcal{I}(k, q) \) by \( \mathcal{I}(k, k^2) \) gives

\[
\mathcal{I}(k, k^2) = \int_0^\infty \frac{dk^2}{2\alpha \mathcal{R}(k, k^2)} \mathcal{I}(k, k^2) \mathcal{S}
\]

and

\[
\frac{1}{2} \mathcal{I}(k, k^2) = \frac{\pi}{V} \sum_{J=1}^{\infty} \delta(k - q) \delta\left(\frac{k^2 + q^2}{2} - \omega^2\right) \mathcal{S}
\]

For a low energy positron, the plasmon contribution in (8-15) can be dropped since the argument of the energy delta function cannot be zero. For instance, for beryllium \( \mathcal{R} \sim 11 \text{ eV} \); while for aluminium it is \( \sim 14 \text{ eV} \).
Formula for the rate of energy loss.

To interpret (8-16) it is convenient to re-examine the general expression for the positron propagator. For \( j > q \),

\[
G_j(k; j) = \langle \langle W \rangle \rangle \delta_k(q) F_j(k) \langle W \rangle | W \rangle \Xi i \kappa_j - \frac{\hbar^2}{2m} \tag{8-18}
\]

where \( \xi_j \) is the energy of the electron system in the state \( | W \rangle \).

But the absolute value squared of the amplitude (8-18) is just the probability that if at time \( t = 0 \) the positron-electron system is in a state \( | W, q \rangle \) (\( | W \rangle \) representing the metal and \( | q \rangle \) representing an incoming positron in a plane wave state of momentum \( k \)), then it will still be in this state at a later time \( \tau \). Thus the probability per unit time that the positron will make a transition from the state \( | q \rangle \) to an arbitrary state \( | q + \phi \rangle \) is \( \mathcal{P}(k; \kappa) \).

Dropping the \( q \) summation in (8-17) gives the transition probability per unit time from \( | q \rangle \) to a specific state \( | q + \phi \rangle \).

Hence it is clear that to get a formula for the rate of energy loss \( R_k \), we need to introduce inside the \( q \) summation in (8-17) an energy transfer term \( \kappa^2 - (q^2 + \phi^2) \). Hence

\[
R_k = \frac{1}{2\pi} \int \frac{\Theta(k-\hbar \omega)}{1 + 2 \sqrt{\frac{\kappa}{\xi_j}}} \Omega_j^2 \left( \frac{\text{det} \left[ (\xi_j + \hbar \omega)^2 - \kappa^2 (q^2 + \phi^2) \right]}{\text{det} \left[ (\xi_j + \hbar \omega)^2 - \kappa^2 \hbar^2 \right]} \right)^2 \tag{8-19}
\]

Note that in (8-19) no arbitrary cut-off occurs in the definition of the potential function \( \sqrt{\frac{\text{det} \left[ (\xi_j + \hbar \omega)^2 - \kappa^2 (q^2 + \phi^2) \right]}{\text{det} \left[ (\xi_j + \hbar \omega)^2 - \kappa^2 \hbar^2 \right]}} \). This formula could be made the basis of the numerical evaluation of \( R_k \). It is felt that this is not really necessary. Instead we approximate \( \sqrt{\frac{\text{det} \left[ (\xi_j + \hbar \omega)^2 - \kappa^2 (q^2 + \phi^2) \right]}{\text{det} \left[ (\xi_j + \hbar \omega)^2 - \kappa^2 \hbar^2 \right]}} \) by \( U(q) \), the screened coulomb...
potential used in LW-I. (This is essentially the approximation of replacing \( g(q; (4)_{\alpha} - \frac{1}{2}) \) by a suitable constant.) Then (8-19) becomes

\[
R_k = 2 \sqrt{\frac{\pi}{k f \Delta k}} \frac{U'}{U} \left( \frac{k^2 - (k + \Delta k)^2}{(k + \Delta k)^2 - k^2 - (k + \Delta k)^2 + k_f^2} \right),
\]

with \( U(k) = \frac{4\pi e^2}{(q^2 + k^2)} \) (\( q \) is the screening parameter of LW-I).

We must now reintroduce \( \Delta k \) and \( \Delta m \) which were set equal to 1. This gives

\[
R_k = \frac{e^2}{(\hbar c)^2} \frac{k_f^2}{k_f} I
\]

with

\[
I = \int \frac{d^2k_1 k_1^3}{(k_1^2 + \beta^2)^2} \left( \frac{1}{(q^2 - (k_1^2)^2)} \right) \left( (q - k_1^2 - q^2 - 2k^2 - (k_1^2 - k_f^2)^2) \right),
\]

where \( \beta = \frac{\Delta k_f}{k_f}, \ \gamma = \frac{\Delta m}{k_f} \), and all other moments are also measured in units of \( k_f \). In the next section \( I \) is evaluated and found to be \( F(\beta) (\frac{\beta^2}{\gamma}) \gamma \Delta k \), where \( F(\beta) \) is as defined in LW-I.

Hence \( R_k = \frac{e^2}{(\hbar c)^2} \Delta k \gamma F(\beta) \), which is formula (1) of LW-I.

Evaluation of integral (8-21).

The following integral is to be evaluated:

\[
I = \int \frac{d^2k_1 d^2k_2}{(k_1^2 + \beta^2)^2} \frac{V(q)}{q^2 + 2q \cdot k_1} \left( (q - k_1^2 - q^2 - 2k^2 - (k_1^2 - k_f^2)^2) \right),
\]

where \( V(q) \Delta k/\left(q^2 + k_f^2\right) \). Since \( q^2 - (k_1^2)^2 > 0 \), a necessary condition for the delta function to contribute is that \( q^2 - (k_1^2)^2 > 0 \). This condition simply states that in an arbitrary energy conserving collision with one of the valence electrons, the positron loses
energy. A more convenient form of the inequality $r^2 - (q^2 + \mu^2) > 0$ is

$$-\mu^2 + \mu^2 > 0 \quad \text{or} \quad \mu^2 > \mu^2$$

where $\mu$ is the cosine of the angle between $\mathbf{q}$ and $\hat{\mathbf{q}}$. Since the maximum value $\mu$ can have is 1, $\mathbf{q}$ is restricted to the interval $(0, \pi)$. Also, for a fixed $\mathbf{q}$, $\mu$ is bounded by $\frac{1}{r}$. Imposing these restrictions on the range of the $\mu$ integration yields

$$I = \pi \int_0^{2\pi} \frac{d\phi}{2\pi} \int_0^\pi \frac{d\mu}{2\pi} (-\mu^2 + 2\mu^2 r \cos \theta) \left[ \delta^2 (q^2 - r^2 + q^2 - \mu^2) \right].$$

The "z-axis" for the $\mu$ integration has been implicitly taken to be along the direction of $\mathbf{q}$. Noting that the argument of the delta function can be reduced to $-\mathbf{q}^2 + 2\mathbf{q}^2$, the integral $I$ can be rewritten as

$$I = \pi \int_0^{2\pi} \frac{d\phi}{2\pi} \int_0^\pi \frac{d\mu}{2\pi} \left[ \delta^2 (q^2 - r^2 + q^2 - \mu^2) \right].$$

Next keep $\mathbf{q}$ fixed and carry out the $\mu$ integration. For this integration, take the z-axis in the direction of the vector $\mathbf{q}$. Then if $\mu'$ denotes the cosine of the angle between $\mathbf{q}$ and $\mathbf{q}'$, the integral $I$ takes the form

$$I = \pi \int_0^{2\pi} \frac{d\phi}{2\pi} \int_0^\pi \frac{d\mu'}{2\pi} \left[ \delta^2 (q^2 - r^2 + q^2 - \mu'^2) \right].$$

The restrictions $|q^2 - r^2| < 1$, $q' > 1$, and $\mu' \leq \mu$ on the $\mu'$ integration can best be visualized by reference to figure 8-5. Two spheres of unit radius are drawn, the first centered at the origin while
the second is displaced an amount $|q_1|$ in the $q$ direction. Since $|q_1| < 2p < 2$, the two spheres always overlap. The two conditions $|q' - q_1| < 1$ and $q' > 1$ are satisfied if and only if $q'$ lies in the shaded region as indicated. Recall that for a fixed $q$, $q'$ can lie only in the interval $q/2$ to $p$, with $p < 1$. If then the directed segment $|q'\mu|$ is drawn extending from the origin along the direction of the vector $q$, it must end somewhere between the two solid lines shown. Now the delta function "clicks" only when the projection of $q'$ on $q$ is equal to the value $q\mu$. So for a contribution $q'$ must be further restricted to a ring, in the plane $\mathcal{A}$, of inner radius $<1-(p\mu)^2/2$ and outer radius $<1-(p\mu-q'\mu)^2$. The plane $\mathcal{A}$ is defined as the plane with normal along the direction of $q$ and a distance $p\mu$ from the origin. Hence we get a
contribution only when \( |q'| \) is in the range \((1, 1 + 2q' \mu - q^2)\), and

\[
J = \int \int \int_{\frac{q^2 - 1 - q^2}{2q}} q^{12} dq' dq \frac{1}{\sqrt{b'^2 - q'^2}} S(2q'(m' - m))\]  

(8-26)

where \( J \) is defined by

\[
J = \int \int \int_{q'^2 < 1} q^{12} dq' dq \frac{1}{\sqrt{b'^2 - q'^2}} S(2q'(m' - m)).
\]

(8-27)

In integral (8-26), the \( q' \) integration was performed. Note that the limits \((q'^2 - 1), \frac{1}{2q}\) and 1 on the \( \mu' \) integration ensure that \( q' \) is in the shaded region of figure 8-5. Finally, in integral (8-26), setting \( a = 2q' \mu \) gives

\[
J = \int \int \int_{1 < q'^2 < 1 - q^2} q^{12} dq' dq \frac{1}{\sqrt{b'^2 - q'^2}} S(x - 2q' \mu).
\]

(8-28)

But

\[
\int_{q'^2 - 1 - q^2}^{2b'} dq \ S(x - 2q' \mu) = 1
\]

(8-29)

because the \( q, \mu, \) and \( t' \) integration ranges have been precisely restricted so as to have \( \mu \) take on the value \( 2q' \mu \) as it ranges over the interval \((q'^2 - 1, q'^2, \frac{1}{2q'})\). Hence

\[
J = \int \int \int_{q'^2 < 1} q^{12} dq' dq = \frac{\pi}{2q} (2q' \mu - b^2).
\]

(8-30)

Substituting expression (8-30) for \( J \) into equation (8-25) for \( I \) and doing the \( q' \) integration yields
The \( \mu \) integration is trivial and

\[
I = \pi \int_0^{\infty} \frac{q^2}{(q^2 + \pi^2)^2} \left( -\frac{q^2 + 2p^2}{6p} \right)^3 \, dq
\]

\[
= \frac{\pi^3}{6p} \left[ \alpha p^3 \left( -\frac{5}{6} + \frac{5}{3} \left( \frac{q}{\pi} \right)^2 + (1 - \frac{5}{3(\pi^2)^2}) \ln \left( 1 + \frac{q}{\pi^2} \right) \right) \right. \\
\left. - \alpha \left( \frac{q}{\pi} \right)^3 \ln^{-1} \left( \frac{q}{\pi} \right) \right].
\]  

Introducing the parameter \( \alpha = \frac{q}{\pi} \), as Lee-Whiting did, gives

\[
I = \frac{\pi \alpha^3}{6} \left\{ \frac{5}{9} \alpha^2 - \frac{5}{3} \alpha + (4 - \frac{5}{9}) \ln \left( 1 + \alpha^2 \right) + \frac{1}{\alpha} \left( \frac{5}{3} \right) \ln^{-1} \alpha \right\}.
\]
Appendix I

Approximate Solution of the Integral Equation for the Local Part of the Effective Potential

Introducing "Fourier transforms" into the integral equation (3-1), the second term on the right becomes

\[
- \frac{i \omega}{V^2} \int \frac{d\omega}{2\pi} \frac{e^{-i\omega(t+t')}}{v(t')} \int \frac{dk}{2\pi} \frac{e^{ikx}}{e^{ikb}} \int \frac{d\omega}{2\pi} C_{\omega}^0 (k, \xi) C_{\omega}^0 (k', -\omega) U(k_m; a', \omega) x
\]

where use was made of equation (A1-1). In (A1-1), k and k' are restricted to the first Brillouin zone, while \( \xi \) and \( \xi' \) are unrestricted; \( k_m \) is an inverse lattice vector, and \( \xi \) and \( \xi' \) are band indices. The delta functions \( \delta[-\xi + \xi'] \delta[1+\xi] \) and \( \delta[-\xi' + \xi'] \delta[1+\xi] \) tell us that \( k_m = [\xi - \xi'] \) and that \( \xi \) and \( \xi' \) must differ only by an inverse lattice vector \( k_m' \). Hence the \( \xi' \) summation in (A1-1) can be done and the \( \xi' \) summation changed to one over only the \( k_m' \)'s. Thus (A1-1) becomes

\[
- \frac{i \omega}{V^2} \int \frac{d\omega}{2\pi} \frac{e^{-i\omega(t+t')}}{v(t')} \int \frac{dk}{2\pi} \frac{e^{ikx}}{e^{ikb}} \int \frac{d\omega}{2\pi} C_{\omega}^0 (k, \xi) C_{\omega}^0 (k', -\omega) U(k_m; a', k_m', \omega) x
\]

Hence the "Fourier transform" of the effective potential satisfies

\[
U(k_m; a', \omega) = \delta_{k_m, 0} \sigma_{\omega}^f
\]
This is an infinite set of coupled integral equations for the effective potential. To get the equation satisfied by the local part, set $\chi_m = 0$. Thus

\[
\psi(0; \vec{q}, \omega) = \psi(0) - \frac{2i}{V} \sum_{k} \frac{d}{d\omega} G_{\xi|\xi}^{E}(\vec{k}; \omega) G_{\xi|\xi}^{E}(\vec{k} - \vec{q}; \omega) \psi(\chi_n; \vec{k} + \chi_n, \omega),
\]

\[
\psi(\chi_n; \vec{k} + \chi_n, \omega) (\vec{k} + \chi_n + \chi_n, \omega) (\vec{k} - \vec{q}, \omega).
\]

In (Al-4) the local part of the effective potential is still coupled on the right hand side to the non-local components. If this coupling is neglected, equation (Al-4) can readily be solved, giving

\[
\psi(0; \vec{q}, \omega) = \psi(0) \left[ 1 + \frac{2i}{V} \sum_{k} \frac{d}{d\omega} G_{\xi|\xi}^{E}(\vec{k}; \omega) G_{\xi|\xi}^{E}(\vec{k} - \vec{q}; \omega) (\vec{k} - \vec{q}, \omega) \right]^{-1}.
\]

Introducing a dielectric constant $\varepsilon(\vec{q}; \omega)$ in (Al-5), it can be rewritten as

\[
\psi(0; \vec{q}, \omega) = \psi(0) / \varepsilon(\vec{q}; \omega)
\]

with

\[
\varepsilon(\vec{q}; \omega) = 1 + \frac{2i}{V} \sum_{k} \frac{d}{d\omega} G_{\xi|\xi}^{E}(\vec{k}; \omega) G_{\xi|\xi}^{E}(\vec{k} - \vec{q}; \omega) (\vec{k} - \vec{q}, \omega) \left[ 1 + \frac{2i}{V} \sum_{k} \frac{d}{d\omega} G_{\xi|\xi}^{E}(\vec{k}; \omega) G_{\xi|\xi}^{E}(\vec{k} - \vec{q}; \omega) (\vec{k} - \vec{q}, \omega) \right]^{-1}.
\]
In the first formula of this appendix we made use of the rule

\[ \Gamma = \int_{\text{crystals}} d^3 \mathbf{x} \; \psi^*_{\mathbf{k}l}(\mathbf{x}) \; \Omega^{-i \mathbf{k} \cdot \mathbf{x}} \; \psi_{\mathbf{k}'l'}(\mathbf{x}) = \sum_{\mathbf{k}'-\mathbf{k}-\mathbf{q}} \Omega_{\mathbf{k}'-\mathbf{k}-\mathbf{q}} \langle \mathbf{k}'l' | \mathbf{k}l \rangle \tag{A1-1} \]

where by definition

\[ (\mathbf{k}'l' | \mathbf{k}l) = \frac{1}{V} \int_{\text{cell}} u^*_{\mathbf{k}'l'}(\mathbf{q}) \; u_{\mathbf{k}l}(\mathbf{q}) \; d^3 \mathbf{q} \]

and \( \mathbf{k}'-\mathbf{k}-\mathbf{q} \) stands for the reduced part of the vector \( \mathbf{k}'-\mathbf{k} \). This statement is well known from solid state theory and a proof will not be given here.
Appendix 2

Variation of the Partial Annihilation Rate with Momentum in the
High Density Limit

When the total momentum \( \mathbf{p} \) of the annihilating pair is smaller than the Fermi momentum, the partial annihilation rate in the high density limit is given by equation (3-11). The singularities of the integrand as a function of the complex variable \( \omega \) are shown in figure A2-1. These consist of the singularities of the effective potential with two additional simple poles at \( \omega = k^2 - i\gamma \) and \( \Omega^2 - (\xi - \omega)^2 + i\gamma \).

Figure A2-1

Since there are no singularities in the first and third quadrants, the integral along the real axis can be changed to one along the imaginary axis without having to introduce any correction term. The proper contour \( \mathcal{C} \) needed to make this change is also shown in figure A2-1. The integral along the two quarter circles does not contribute since for \( |\omega| \rightarrow \infty \) the integrand behaves at least like \( 1/\omega^2 \). Thus the integral along the real axis equals the integral along the imaginary axis; i.e.

\[
\int \text{d} \mathbf{p} \rightarrow \int \text{d} \mathbf{p} \text{Im} \mathcal{C}
\]
\[ \Theta^{(1)}_{\epsilon c} = \frac{2i}{\sqrt{2}} \int_{0}^{1} \frac{d\nu}{2\pi} \frac{u(k;\nu)}{k^2 - (q-k)^2 - i\nu} \Theta(\mu - k_1 - p) . \quad (A2-1) \]

Since \( u(k;\nu) = u(-k;\nu) \), the range of the \( \omega \) integration in \((A2-1)\) can be restricted to \((0, +\infty)\). Hence

\[ \Theta^{(1)}_{\epsilon c} = -\frac{2i}{\sqrt{2}} \int_{0}^{1} \frac{d\omega}{2\pi} \frac{u(k;\omega)}{(k^2 - (q-k)^2 - 2\omega^2)} \frac{2k^2[(q-k)^2] - 2\omega^2}{(k^2 + \omega^2)[(p^2 - (q+k)^2 + \omega^2)]} . \quad (A2-2) \]

Change the \( \sum \) summation in \((A2-2)\) to an integration and choose the \( k_3 \) axis along the direction of \( \hat{\epsilon} \). To visualize the restrictions imposed on the \( k \) integration by the inequality \( |q+k| > \rho_F \), refer to figure A2-2. For \( |k| \) in the range \((0, \rho_F - \mu)\), the inequality is violated, while for \( |k| \in (\rho_F - \mu, \rho_F + \mu) \) there can be a contribution provided the direction of \( \mathbf{k} \) is restricted to the cap shown, i.e. \( \mathbf{k} \in \left( \frac{\rho_F^2 - p^2 - k^2}{2\rho_F} \right) \). For \( k > \rho_F \) there are no restrictions at all.

**Figure A2-2**

Restrictions on the \( k \) integration imposed by the inequalities \( |q+k| > \rho_F \) and \( p < \rho_F \).

Hence we have the rule

\[
\begin{align*}
\int_{1/2}^{1} d^3 k & \rightarrow \int_{\rho_F}^{\rho_F + \mu} d^3 q \int_{0}^{2\pi} d\theta_q \int_{0}^{\rho_F} d\rho_q \int_{0}^{\rho_F} d\rho_q \int_{0}^{2\pi} d\phi_q \int_{0}^{2\pi} d\phi_q \left\{ \int_{k^2 + \omega^2}^{\infty} d\omega \right\}^{3} \frac{2k^2[(q-k)^2] - 2\omega^2}{(k^2 + \omega^2)[(p^2 - (q+k)^2 + \omega^2)]} , \quad \rho_F = \frac{\varphi \epsilon}{p^2} . \quad (A2-3)
\end{align*}
\]
Applying this rule to \((A2-2)\) gives

\[
\rho_{\text{tot}}^{(1)} = -\frac{2\lambda}{V} \int_{0}^{2\pi} d\phi \int_{0}^{\infty} k^2 dk \int_{0}^{\infty} \frac{d\omega}{\omega} \frac{u(k;\iota\omega)}{(\omega^2 + k^2)^{2}} \frac{k^2 - 2\pi \mu - k\omega}{(k^2 + \omega^2 + \mu^2)^{2}}
\]

\[\tag{A2-9}\]

But

\[
\int \frac{dk}{k^2 + \omega^2 + \mu^2} = \frac{1}{\omega} \, \text{tan}^{-1} \left( \frac{k^2 + \omega^2}{\mu^2} \right) + \text{const}. \tag{A2-5a}\]

and

\[
\int \frac{dk}{\mu^2 + \omega^2 + \mu^2} = \frac{1}{\omega} \, \text{tan}^{-1} \left( \frac{\mu^2 + \omega^2}{\omega^2 + \mu^2} \right) + \text{const}. \tag{A2-5b}\]

Using \((A2-5a)\) and \((A2-5b)\) in \((A2-4)\), it becomes

\[
\rho_{\text{tot}}^{(1)} = -\frac{2\lambda}{V} \int_{0}^{2\pi} d\phi \int_{0}^{\infty} k^2 dk \int_{0}^{\infty} \frac{d\omega}{\omega} \frac{u(k;\iota\omega)}{(\omega^2 + k^2)^{2}} \frac{k^2 - 2\pi \mu - k\omega}{(k^2 + \omega^2 + \mu^2)^{2}} \left[ \text{tan}^{-1} \left( \frac{k^2 + \omega^2}{\mu^2} \right) - \text{tan}^{-1} \left( \frac{\mu^2 + \omega^2}{\omega^2 + \mu^2} \right) \right]
\]

\[\tag{A2-6}\]

\[
-\frac{2\lambda}{V} \int_{0}^{\infty} k^2 dk \int_{0}^{\infty} \frac{d\omega}{\omega} \frac{u(k;\iota\omega)}{(\omega^2 + k^2)^{2}} \frac{k^2 - 2\pi \mu - k\omega}{(k^2 + \omega^2 + \mu^2)^{2}} \left[ \text{tan}^{-1} \left( \frac{k^2 + \omega^2}{\mu^2} \right) - \text{tan}^{-1} \left( \frac{\mu^2 + \omega^2}{\omega^2 + \mu^2} \right) \right]
\]

In \((A2-6)\) make the transformation \(\omega \to \mu \omega\); then measure all momenta in units of \(p_{F}\) and send \(\omega \to \omega p_{F}\). Finally introduce the parameter \(\alpha = 1/(\pi^2 p_{F}^2) = \alpha_{0}/(1.91 \, \pi^2)\). This gives

\[
\rho_{\text{tot}}^{(1)} = -\frac{2\lambda}{V} \int_{0}^{2\pi} d\phi \int_{0}^{\infty} k^2 dk \int_{0}^{\infty} \frac{d\omega}{\omega} \left( \frac{2}{k^2 + \omega^2 + \mu^2} \right) \left( k \text{ln} \left( \frac{\omega^2 + (k + \mu)^2}{\omega^2 + (k - \mu)^2} \right) + \omega \left( \text{tan}^{-1} \frac{k^2 + \omega^2}{\mu^2} - \text{tan}^{-1} \frac{\mu^2 + \omega^2}{\omega^2 + \mu^2} \right) \right)
\]

\[
\rho_{\text{tot}}^{(1)} = -\frac{2\lambda}{V} \int_{0}^{2\pi} d\phi \int_{0}^{\infty} k^2 dk \int_{0}^{\infty} \frac{d\omega}{\omega} \left( \frac{2}{k^2 + \omega^2 + \mu^2} \right) \left( k \text{ln} \left( \frac{\omega^2 + (k + \mu)^2}{\omega^2 + (k - \mu)^2} \right) + \omega \left( \text{tan}^{-1} \frac{k^2 + \omega^2}{\mu^2} - \text{tan}^{-1} \frac{\mu^2 + \omega^2}{\omega^2 + \mu^2} \right) \right)
\]
\[
\frac{\sqrt{\pi}}{V} \int_{k_F}^{1} \frac{d k}{k^2} \int_{0}^{\infty} \frac{d \omega}{
abla + \Omega} G(k, \omega) \left( \frac{1}{k^2 \omega^2} \left[ \frac{1}{\Lambda^2 (\omega^2 + (k \Lambda)^2)} + \frac{1}{\Lambda (\omega^2 + (k \Lambda^2))^2} \right] + \frac{1}{\Lambda (\omega^2 + (k \Lambda^2))^2} \right) \right) \] (A2-1)

with

\[G(k, \omega) = \frac{2}{k_F} G(k, \omega) \] (A2-2a)

The function \(G(k, \omega)\) on the right hand side of (A2-2) is defined as an integral in (3-13). This integral is quite familiar and we will simply state the result here:

\[G(k, \omega) = 2 \pi \left[ 1 - \frac{1}{2} (1 - \frac{1}{4} (k^2 \omega^2)) \right] \frac{1}{\omega^2 + (k \Lambda^2)^2} \frac{1}{\Lambda^2 \Lambda^2 \Lambda^2 + \Lambda^2} \] (A2-2b)

In the form (A2-7), \(\tilde{\kappa}^2 \) was evaluated on the Toronto IBM 7090 computer. The \(\omega\) integration was done first for fixed \(k\), using 371 points (Simpson's rule). In this way a table of the integrand for the \(k\) integration was constructed. The increment used on the \(k\) variable depended on the actual value of \(k\). For instance, for \(k < \Lambda\) it was fixed at 0.01 while for \(k > \Lambda\) we used 1.0. The results for three values of momentum and two values of \(\tilde{\kappa}\) are given in Table A2-1.

<table>
<thead>
<tr>
<th>(\tilde{\kappa})</th>
<th>(\tilde{k} d=1)</th>
<th>(\tilde{k} d=2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>1.098</td>
<td>2.060</td>
</tr>
<tr>
<td>0.5</td>
<td>1.164</td>
<td>2.181</td>
</tr>
<tr>
<td>0.9</td>
<td>1.497</td>
<td>2.628</td>
</tr>
</tbody>
</table>

Momentum dependence of the partial annihilation rate in the high density limit. The variable \(\tilde{\kappa}\) is momentum in units of \(k_F\) and the parameter \(\tilde{\kappa}\) is related to \(\kappa\) by \(\tilde{\kappa} = \kappa / (1917 \pi^2)\).
For comparison suppose the effective potential in (3-11) is replaced by its static limit \( \chi(\xi;\omega) \); then \( \Theta^{(0)}_{\text{p}e} \) becomes

\[
\Theta^{(0)}_{\text{p}e} = \frac{2\pi i}{V} \int_\mathbb{R} \left[ \frac{d\omega}{2\pi} \, \chi(\xi;\omega) \, \frac{1}{k^2 - \omega + i\eta} \, \frac{\Theta(\xi + \xi - p_e)}{p^2 - (\xi + \xi)^2 + k^2 - p^2} \right].
\]

(A2-9)

Thus

\[
\Theta^{(0)}_{\text{p}e} = \frac{2\pi i}{V} \int_\mathbb{R} \chi(\xi;\omega) \, \frac{\Theta(\xi + \xi - p_e)}{(\xi + \xi)^2 + k^2 - p^2}.
\]

(A2-10)

Table A2-2 below gives \( \Theta^{(0)}_{\text{p}e} \) for various values of \( \eta \).

<table>
<thead>
<tr>
<th>( \eta = \eta_{\text{p}e} )</th>
<th>( \Theta^{(0)}_{\text{p}e} )</th>
<th>( \Theta^{(0)}_{\text{p}e} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( 1 )</td>
<td>1.991</td>
<td>1.755</td>
</tr>
<tr>
<td>( 3 )</td>
<td>1.005</td>
<td>1.771</td>
</tr>
<tr>
<td>( 5 )</td>
<td>1.035</td>
<td>1.805</td>
</tr>
<tr>
<td>( 7 )</td>
<td>1.086</td>
<td>1.865</td>
</tr>
<tr>
<td>( 8 )</td>
<td>1.125</td>
<td>1.909</td>
</tr>
<tr>
<td>( 9 )</td>
<td>1.179</td>
<td>1.972</td>
</tr>
</tbody>
</table>

Momentum dependence of the partial annihilation rate in the high density limit when the effective potential \( \chi(\xi;\omega) \) is replaced by its static limit \( \chi(\xi;\omega) \).

**Total annihilation rate**

Changing the integral along the real axis in (3-12) to one along the imaginary axis, the total annihilation rate in the high density limit becomes
\[ \theta^{(0)} = \frac{2 \lambda}{\sqrt{\beta}} \int \frac{d \omega}{2 \pi} u(k; i\omega) q(k; i\omega) \frac{2k^2}{k^2 + \omega^2}. \quad (A2-11) \]

By making a series of substitutions identical to those carried out on \( \theta^{(0)} \), it is not difficult to show that

\[ \theta^{(1)} = \theta^{(0)} \cdot 6 \int_0^\infty k^3 dk \int_0^\infty \frac{d \omega}{2 \pi} \frac{1}{k^2 + \omega^2} \frac{\alpha \phi(k; \omega)}{k^2 + \alpha \phi^0(k; \omega)}. \quad (A2-12) \]

Numerical evaluation of \((A2-12)\) gives \( \theta^{(0)} = 1.24 \theta^{(0)} \) for \( \alpha = 1 \), and \( 2.19 \theta^{(0)} \) for \( \alpha = 2 \).
Appendix 3

Derivation of the Bethe-Goldstone Equation

Consider the integral equation (3-15) giving the electron-positron propagator

\[ G_p(x', y') = G_e(x', y') G_p(x, y') - \int d^3 p \, G_e(x, y') G_p(x', y') \, \Delta_p(y', p) \, G_p(y, p) \]  \hspace{1cm} (A3-1)

Throughout this appendix it is understood that \( x', y' \), \( x \), etc.

Introduce a Bethe-Goldstone amplitude according to the prescription

\[ G_p(x', y') = \int d^3 p \, \Delta(x, p) \, G_e(x, y') \, G_p(y, p) \]  \hspace{1cm} (A3-2)

Writing the correlation function in the particular form (A3-2) is clearly consistent as can be established from the iterated solution of (A3-1). Introducing equation (A3-2) into (A3-1), one finds that the amplitude \( \Delta(x', y') \) must satisfy the equation

\[ \Delta(x', y') = \Delta(x, y') \Delta(x', y') - \int d^3 p \, \Delta(x, p) \, G_e(x, y') \, \Delta(y, p) \, \Delta(y', p) \]  \hspace{1cm} (A3-3)

Write the space part of the Fourier transform of \( \Delta(x', y') \) as

\[ \Delta(x', y') = \sum_{m} \Delta_{m, m'} (x', y') \]  \hspace{1cm} (A3-4)

Making use of (A3-4), equation (A3-3) can be rewritten as

\[ \Delta(\mathbf{x}', \mathbf{y}') = \sum_{m, m'} \Delta_{m, m'} (\mathbf{x}', \mathbf{y}') - \int \frac{d^3 p}{(2\pi)^3} G_e(p, \mathbf{y}') \, \Delta_{m, m'} (\mathbf{p}, \mathbf{x}') \]  \hspace{1cm} (A3-5)
From the iterated solution of (A3-5) it is obvious that \( \Delta_{m,n}^{(1)} \) can depend only on \( \frac{1}{\gamma} \). Hence we can write

\[
\Delta_{m,n}^{(1)} \left( \frac{1}{\gamma} \right) = \int \frac{d\omega}{2\pi} e^{-i\omega \left( \frac{1}{\gamma} \right)} \Delta_{m,n}^{(1)} (\omega). \tag{A3-6}
\]

Doing the time Fourier transformation of (A3-5), it becomes

\[
\Delta_{m,n}^{(1)} (\omega) = S_{m,n} S_{m,n} - i \sum_{y} u(y; 0) \int \frac{d\epsilon}{2\pi} C_{e}^{(m,n)}(\epsilon) C_{f}^{(m,n)}(\omega - \epsilon) \Delta_{m,n}^{(1)} (\epsilon). \tag{A3-7}
\]

Next we need an expression for the contribution of (A3-1) to the partial annihilation rate \( \Theta_{f} \) involving the amplitude \( \Delta \) rather than the correlation function \( G_{CP} \). This is achieved by substituting (A3-2) into the expression for \( \Theta_{f} \) and Fourier transforming,

\[
\Theta_{f} = -i \sum_{m,n} \int \frac{d\omega}{2\pi} \Delta_{m,n}^{(1)} (\omega) \int \frac{d\epsilon}{2\pi} C_{e}^{(m,n)}(\epsilon) C_{f}^{(m,n)}(\omega - \epsilon). \tag{A3-8}
\]

But it is easy to verify that

\[
\int \frac{d\epsilon}{2\pi} C_{e}^{(m,n)}(\epsilon) C_{f}^{(m,n)}(\omega - \epsilon) = i \left[ \rho_{m,n}^{+} (\omega) + \rho_{m,n}^{-} (\omega) \right]. \tag{A3-9}
\]

with

\[
\rho_{m,n}^{+} (\omega) = \frac{\theta(m - n) \theta(n)}{m^2 + n^2 - \omega - i\eta} \quad \text{and} \quad \rho_{m,n}^{-} (\omega) = \frac{-\theta(m - n) \theta(-n)}{m^2 + n^2 - \omega + i\eta}. \tag{A3-10}
\]

Hence equations (A3-7) and (A3-8) become respectively

\[
\Delta_{m,n}^{(1)} (\omega) = S_{m,n} S_{m,n} + i \sum_{y} u(y; 0) \left( \rho_{m,n}^{+} (\omega) + \rho_{m,n}^{-} (\omega) \right) \Delta_{m,n}^{(1)} (\omega). \tag{A3-11}
\]
At this point it would be possible to read from equation (A3-11) the analytic properties of the amplitude $\Lambda_{m_0\omega_1}$ as a function of the complex variable $\omega$ and then use this knowledge to carry out the $\omega$ integration in (A3-12). This would be a very elegant way to proceed but inevitably leads to integrals around cuts which, to evaluate, require a knowledge of $\text{Im} \Lambda(\omega)$ across these cuts. To avoid this we will reduce (A3-11) and (A3-12) further before attempting the integration. However, our method will rely heavily on perturbation theory. To simplify the manipulations, it is convenient to introduce a formal matrix notation. In this notation (A3-11) and (A3-12) take the form

$$\langle m_0 | \Lambda(\omega) | m_1 \rangle = 1 + \langle P^+(\omega) + P^-(\omega) | U \Lambda(\omega) | m_1 \rangle$$  \hspace{1cm} (A3-13)$$

$$\Theta_f = -\frac{i}{\hbar} \sum_{m_0}^{m} \sum_{m_1}^{m+1} \delta_{m_0, m_1} \int \frac{d\omega}{2\pi} \langle m_0 | \Lambda(\omega) | m_1 \rangle \langle P^+(\omega) + P^-(\omega) | u \rangle$$  \hspace{1cm} (A3-14)$$

where

$$\langle m_0 | u | m_1 \rangle = \frac{1}{\sqrt{2}} \sum_{q=0}^{2} \langle u | q; 0 \rangle S_{m_0, q} S_{m_1, q} \psi_0 \psi_0$$

$$\langle m_0 | \Lambda(\omega) | m_1 \rangle = \Lambda_{m_0 m_1 \omega} \omega$$

$$\langle m_0 | P(\omega) | m_1 \rangle = P_{m_0 m_1 \omega} \omega$$

$$\langle m_0 | S | m_1 \rangle = S_{m_0 m_1} \omega$$

Substituting the iterated solution of (A3-13) into the expression
\( \Lambda (p^+ p^-)^* \) and concentrating on the \( n \)th order term in this expansion, we obtain

\[
(p^+ p^-) u (p^+ p^-) u \cdots (p^+ p^-) u (p^+ p^-) .
\]  

(A3-15)

Expression (A3-15) can be expanded further in \((m^2)^2\) products, a possible member being

\[
p^+ u p^+ u \cdots p^+ u p^+ .
\]  

(A3-16)

As a function of the complex variable \( \omega \), expression (A3-16) is analytic in the upper half plane. Hence, when the integration over \( \omega \) (required to determine the contribution to the partial annihilation rate from (A3-16)) is carried out we get zero. Another possible product is (A3-16) with one of the \( p^+ \) replaced by a \( p^- \). In fact, there are \( m+2 \) such products, namely

\[
\begin{bmatrix}
p^+ u p^+ u p^+ \cdots p^+ u p^+ \\
\vdots \\
p^+ u p^+ u \cdots p^+ u p^-
\end{bmatrix}^{m+1}
\]  

(A3-17)

If an intermediate amplitude \( \Lambda^0 \) and its conjugate \( \Lambda^{0\dagger} \) are introduced by

\[
\Lambda^0 = 1 + p^+ u \Lambda^0 \quad \text{and} \quad \Lambda^{0\dagger} = 1 + \Lambda^{0\dagger} u p^+ \]  

(A3-18)

then clearly the \( n \)th order term in the expansion of \( \Lambda^0 p^- \Lambda^{0\dagger} \) is just (A3-17). Thus, provided that only the terms (A3-17) in the expansion of \( \Lambda (p^+ p^-) \) contribute to the partial annihilation rate \( \bar{\rho} \), \( \Lambda (p^+ p^-) \) can be replaced by \( \Lambda^0 p^- \Lambda^{0\dagger} \). That is, instead of (A3-11) and (A3-12) we can write

\*(Integrating \( \Lambda (p^+ p^-) \) over \( \omega \) essentially gives \( \bar{\rho} \).)*
\[ \Omega_{\mathbf{m}, \mathbf{m}'; \mathbf{m}''}^{\alpha}(\omega) = S_{\mathbf{m}, \mathbf{m}'} S_{\mathbf{m}', \mathbf{m}''} + \frac{1}{4} \sum_{\mathbf{t}} \frac{u(t; \beta)}{u(t; \alpha)} \Delta_{\mathbf{m}, \mathbf{m}'}^{\alpha}(\omega) \Delta_{\mathbf{m}', \mathbf{m}''}^{\beta}(\omega), \]  

\[ \Omega_{\mathbf{m}, \mathbf{m}'; \mathbf{m}''}^{\alpha +}(\omega) = S_{\mathbf{m}, \mathbf{m}'} S_{\mathbf{m}', \mathbf{m}''} + \frac{1}{4} \sum_{\mathbf{t}} \frac{u(t; \beta)}{u(t; \alpha)} \Delta_{\mathbf{m}, \mathbf{m}'}^{\alpha +}(\omega) \Delta_{\mathbf{m}', \mathbf{m}''}^{\beta}(\omega), \]  

and

\[ \theta_{\mathbf{p}} = \frac{i}{\sqrt{\pi}} \int_{-\infty}^{\infty} S_{\mathbf{p}, \mathbf{m}+\mathbf{m}} S_{\mathbf{p}', \mathbf{m}'+\mathbf{m}''} \frac{1}{2} \int_{M} \frac{d\omega}{\omega} \Delta_{\mathbf{m}, \mathbf{m}'}^{\omega}(\omega) \Delta_{\mathbf{m}', \mathbf{m}''}^{\omega}(\omega) \Delta_{\mathbf{m}, \mathbf{m}'}^{\omega}(\omega), \]  

Finally, in order to convince ourselves that only the terms (A3-17) in the expansion of (A3-15) can contribute to \( \theta_{\mathbf{p}} \), we note that all the terms left out must contain at least two factors \( \mathcal{P}(\omega) \), i.e. two positron theta functions of the form \( \Xi(\omega) \). But such a theta function can be used to carry out a momentum summation, leaving a volume factor \( 1/V \) without a corresponding momentum summation. This leads to terms of the order \( 1/V \) as compared to the terms (A3-17), and so these must vanish in the limit of infinite volume. In other words, all these terms are proportional to at least the first power of the positron density in the system, which is zero.

As functions of the complex variable \( \omega \), the amplitude \( \Omega^0(\omega) \) and its conjugate \( \Omega^1(\omega) \) are analytic in the upper half plane with a cut extending from \( \mathcal{P}_{\mathbf{p}} \) to \( +\infty \) just below the real axis. There is also an extra simple pole falling somewhere on this cut. The analytic properties of the integrand in equation (A3-20) are shown in figure A3-1. These are just the singularities of the Bethe-Goldstone amplitude with an additional simple pole at \( \omega = m' + \gamma \) coming from \( \mathcal{P}_{\mathbf{p}, \mathbf{m}'} \). Completing the contour above, equation (A3-20) becomes
where use was made of the fact that \( \mathbf{m} + \mathbf{m}' = \mathbf{m}'' + \mathbf{m}''' \) (ensured by the translational invariance of the theory). Note that closing the contour above is forced on us by the exponential factor \( e^{i\omega_f} \), at least for the case when \( \Lambda^0 \) and \( \Lambda^0 + \) are replaced by their zeroth approximation. (This factor is of course not important for higher order approximations.)

**Figure A3-1**

Singularities of the integrand in (A3-20). The contour is completed above.

Finally, since \( \Lambda^0_{\mathbf{p}_0; \mathbf{m}_0} = \Lambda^0_{\mathbf{m}_0; \mathbf{p}_0} \) we get

\[
\Theta_{\mathbf{p}} = \frac{\Lambda}{V} \Theta(\mathbf{p}_F - \mathbf{p}) \epsilon(\mathbf{p})
\]  

(A3-22)

with

\[
\epsilon(\mathbf{p}) = \left[ \sum_{\mathbf{m}, \mathbf{m}'} S_{\mathbf{m} + \mathbf{m}'; \mathbf{p}} \Lambda^0_{\mathbf{m} + \mathbf{m}'; \mathbf{p}_0} (\mathbf{p}^2)^2 \right]^{-1}
\]  

(A3-23)

where \( \epsilon(\mathbf{p}) \) is called the enhancement factor for an electron of momentum \( \mathbf{p} \). Note that \( \Theta_{\mathbf{p}} = 0 \) for \( \mathbf{p} > \mathbf{p}_F \) and that...
The "\(i\eta\)" factor in the denominator of the second term of the right hand side of (A3-24) was dropped because it cannot have a zero: \(m^2 + m^2 > p_f^2\) while \(p^2 < p_f^2\). 

\[
\Delta_{m^2, m^2}^{a, b} \left( p^2 \right) = \delta_{m^2, p^2} \sum_{a, b} \delta^{ab} \left( p^2 \right) \frac{1}{m^2 + m^2 - p^2} \left( p^2 \right) + \sum_{A} U_{a} \sum_{b} \Delta_{m^2, A}^{A, b} \left( p^2 \right) 
\]
Appendix I

Reduction and Numerical Evaluation of Some Integrals Giving the Effect of Hole-Particle Interactions on the Annihilation Rates

Integral 1.

From equation \((1-14)\) \(I_1\) stands for the integral

\[
I_1 = -\alpha^2 \int_{-1}^{1} \frac{d^2 q \, d^2 p}{(q^2 + p^2 + 1^2 + (q^2 + p^2 + 1^2 + 1^2)^2)} \cdot \tag{A9-2}
\]

Do the \(\theta\) integration first, considering \(\theta\) fixed. Applying the rule \((A2-3)\) to the \(\theta\) integration in \(I_1\), gives

\[
I_1 = -\alpha^2 \int_{-1}^{1} \frac{d^2 q \, d^2 p}{(q^2 + p^2 + 1^2 + (q^2 + p^2 + 1^2 + 1^2 + 1^2)^2)} \cdot \tag{A9-2}
\]

\[
I_1 = -\alpha^2 \left[ \int_{-1}^{1} \frac{d\mu}{\sqrt{b^2 + \mu^2}} \left\{ \int_{-1}^{1} \frac{d\rho}{\sqrt{b^2 + \rho^2 + \mu^2}} \left[ \ln \left( \frac{q^2 + p^2 + 1^2 + 1^2 + 1^2 + 1^2}{b^2 + \mu^2} \right) + \text{const} \right] \right\} \right]. \tag{A9-3}
\]

But

\[
\frac{d\mu}{(q^2 + \mu^2)(q^2 + \mu^2 + 1^2 + 1^2)} = \frac{1}{b^2 - 1^2} \left[ \ln \left( \frac{q^2 + p^2 + 1^2 + 1^2}{b^2 + \mu^2} \right) + \text{const} \right]. \tag{A9-4}
\]

Using \((A4-3)\), the integral \(I_1\) can be rewritten in the form

\[
I_1 = -\alpha^2 \left[ \int_{-1}^{1} \frac{d^2 q \, d^2 p}{\mu^2} \left\{ \int_{-1}^{1} \frac{d\rho}{\sqrt{b^2 + \rho^2 + \mu^2}} \left[ \ln \left( \frac{q^2 + p^2 + 1^2 + 1^2}{b^2 + \mu^2} \right) + \text{const} \right] \right\} \right]. \tag{A9-4}
\]
Finally, integrating over the angles of \( \phi' \) gives a factor of \( \pi \).

Thus

\[
I_1 = - (2\pi v)^2 \int_0^1 dq' U(q') \left[ f_1(q') + f_1(q') \right] \equiv I_1', \quad v \neq 1
\]  

\[
\text{(A1-5)}
\]

with

\[
f_1(q') = \int_0^{\gamma} dq'' \ U(q) \left( \frac{q''}{q'' - q} \right) \frac{2m( q'' + q') ( q'' + q' )}{( q'' + q' ) ( q'' + q' )}
\]

\[
\text{(A1-6)}
\]

**Integral 2.**

From equation (11-15) the integral \( I_2 \) is given by

\[
I_2 = - \alpha^2 \sum_{b} \int_0^{\gamma} dq' \ U(q') \frac{1}{(q'' + \gamma^2 + \gamma'') \left[ (q'' + \gamma^2 + \gamma'') \right]}
\]

\[
\text{(A1-7)}
\]

The region of integration for \( \phi' \) is clearly the same as that for integral \( I_1 \), except that \( \frac{q''}{q'' - q} \) must be cut off at \( 1 \). Hence

\[
I_2 = - \alpha^2 \sum_{b} \int_0^{\gamma} dq' \ U(q') \frac{1}{(q'' + \gamma^2 + \gamma'') \left[ (q'' + \gamma^2 + \gamma'') \right]}
\]

\[
\text{(A1-8)}
\]

But

\[
\int \frac{dq'}{(q'' + \gamma'')(q'' + \gamma')} = \frac{3}{(q'' + \gamma'')(q'' + \gamma') \left[ -2m \left( \frac{q'' + \gamma'}{b'' + \gamma'} \right) + \text{const.} \right]}
\]

\[
\text{(A1-9)}
\]

Thus

\[
I_2 = - (2\pi v)^2 \int_0^1 dq' U(q') F_2(q')
\]

\[
\text{(A1-10)}
\]
with
\[
I_2(b') = \int_{b'}^{1} \frac{\partial^4}{\partial b^4} (1/b) \cdot \frac{1}{2} \left( \frac{1}{b'^2 - b^2} \right) \ln \left( \frac{b'^2 + b^2 + 1}{b'^2 - b^2 + b^2} \right).
\]  
(A4-11)

In the forms (A4-5) and (A4-10) respectively, integrals \( I_1 \) (\( \Sigma_1 + \Sigma_2 \)) and \( I_2 \) were evaluated numerically of the McGill IBM 1410 electronic computer. First the functions \( F_1(b') \), \( F_2(b') \), and \( F_2(b') \) were calculated for 40 values of \( b' \) in the range \((0,1)\). For a given \( b' \) the range of the integral defining each of the three \( F(b') \) functions is fixed. These were calculated using Simpson's rule with the number of points adjusted to the range of \( b' \). For example, in the case of \( F_2(b') \) where \( b' \) ranges from 1 to \( +\infty \), 121 points were used. From a table of the \( F(b') \)'s the \( I_3 \)s are readily determined. The results are given in Table A4-1 below.

<table>
<thead>
<tr>
<th>Table A4-1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Integral</td>
</tr>
<tr>
<td>-------------</td>
</tr>
<tr>
<td>( I_1 )</td>
</tr>
<tr>
<td>( I_2 )</td>
</tr>
<tr>
<td>( I_2 )</td>
</tr>
<tr>
<td>( I_1 + I_2 + I_3 )</td>
</tr>
</tbody>
</table>

Intermediate integrals in the evaluation of \( \mathcal{R}_{1}^{(ab)} \) which gives the effect on the annihilation rates of electron hole-positron interactions (diagram 4-1b).

**Integral 3**

Equation (4-27) gives for \( \Delta \):
The variable \( \xi \) could be kept fixed and the rule (A2-3) applied to the \( \xi \) integration. However it was found that doing the \( \xi' \) integration first leads to a final expression slightly easier to handle numerically. Keep \( \xi \) fixed in the \( z \)-direction for the \( \xi' \) integration and refer to figure A4-1. For \( \xi' \leq 1 \) the

\[ J_1 = \alpha^3 \int_{\xi' > 1} \frac{b^1}{b_{21}} \left[ U(\xi') U'_{\xi'} \right] \frac{1}{b_{21}^2 \left[ b_{21}^2 + 2 \xi_{12}^2 b_{12}^2 \right]} \, d\xi'. \]  

(R4-12)

Figure A4-1

Restrictions on the direction of \( \xi' \), for a fixed \( \xi'' \), imposed by the inequality 

\[ |\xi' + \xi''| > 1. \]

Condition \( |\xi' + \xi''| > 1 \) is satisfied for an arbitrary direction of \( \xi' \).

If \( \xi'' > 2 \) this is the only possible situation since \( |\xi' + \xi''| < 1 \), but if \( \xi'' < 2 \) the range \( \xi'' \in (1, 1/1) \) must be treated separately. In this case the angular integration \( \int_{\xi''} \) must be restricted to the cap shown in figure A4-1, i.e. \( \xi'' \) ranges over \((0,2\pi)\) and \( \xi' \) ranges over \((1-\frac{1}{2}, \frac{1}{2}, 1)\). Hence

\[ J_1 = \alpha^3 \int_{\xi'' > 1} \frac{b_{12}}{b_{21}} \left[ U(\xi') U'_{\xi'} \right] \frac{1}{b_{21}^2 \left[ b_{21}^2 + 2 \xi_{12}^2 b_{12}^2 \right]} \int_{\xi''} \frac{1}{b_{21}^2 \left[ b_{21}^2 + 2 \xi_{12}^2 b_{12}^2 \right]} \, d\xi' \]

\[ + \alpha^3 \int_{\xi'' < 1} \frac{b_{12}}{b_{21}} \left[ U(\xi') U'_{\xi'} \right] \frac{1}{b_{21}^2 \left[ b_{21}^2 + 2 \xi_{12}^2 b_{12}^2 \right]} \int_{\xi''} \frac{1}{b_{21}^2 \left[ b_{21}^2 + 2 \xi_{12}^2 b_{12}^2 \right]} \, d\xi'. \]  

(R4-13)
The \( \mu'_6 \) integration in (A4.1-13) can easily be carried out and then the angular part of the \( \theta \) integration gives simply \( \pi \), so that \( d_1 \) becomes

\[
d_1 = (2\pi)^2 \int_1^2 U(y) \, d_1 \left[ \frac{\partial}{\partial \theta} \left( \frac{y_2 + \frac{1}{2} a_1 a_2}{b} \right) \right] + \int_1^1 U(y) \, d_1 \left[ \frac{\partial}{\partial \theta} \left( \frac{y_2 + \frac{1}{2} a_1 a_2}{b} \right) \right].
\]

\[\text{(A4.1-14)}\]

**Integral \( d_2 \).**

The integral \( d_2 \) is given in formula (4.28), which is

\[
d_2 = \kappa^2 \int \int \frac{U(y) \, U(y')}{b^2 + \frac{1}{2} a_1 a_2 (y_2 - y_2')} \, dy \, dy'.
\]

\[\text{(A4.1-15)}\]

To proceed with the reduction of this integral keep \( \mu'_6 \) fixed. For the \( \theta' \) integration take the \( z \)-axis along the direction of \( \theta' \). Figure A4-2 will help to visualize the situation. The inequalities \( |\theta' + \theta| < \pi \) and \( |\theta' - \theta| \) restrict \( \theta' \) to the range \( (1, 1 + \frac{1}{2} a_1 a_2) \) if \( \theta < \frac{\pi}{2} \), and to the range \( (\frac{\pi}{2} - 1, \frac{\pi}{2} + 1) \) if \( \theta > \frac{\pi}{2} \). For \( \theta' \) in the above ranges the allowed directions of \( \theta' \) must be further restricted to the spherical cap shown in figure A4-2, i.e. \( \theta' \in (\theta, 2\pi), \theta' \in (-\theta, \frac{\pi}{2} - \frac{1}{2} a_1 a_2) \). Hence \( d_2 \) can be written as

\[
d_2 = \kappa^2 \int_1^1 U(y) \, d_1 \left[ \frac{\partial}{\partial \theta} \left( \frac{y_2 + \frac{1}{2} a_1 a_2}{b} \right) \right] + \int_1^1 U(y) \, d_1 \left[ \frac{\partial}{\partial \theta} \left( \frac{y_2 + \frac{1}{2} a_1 a_2}{b} \right) \right].
\]

\[\text{(A4.1-16)}\]
where the integration over $d\Delta \frac{1}{2}$ was also done. Doing the $\mu'$ integration, (Ah-16) becomes

$$j_2 = (\pi\alpha)^2 \int_0^{\infty} U(q) dq \int_0^{\infty} U(q') dq' \frac{1}{b} \text{Re} \left( \frac{\omega^2}{q^2 + q'^2} \right)$$

where $q = q_f$, for $|q_f|$ fixed, imposed by the inequality $|q_f + q'| < 1$.

The numerical evaluation of $j_1$ and $j_2$ was also carried out on the McGill IBM 1401 computer, and the techniques used were identical to those described for the evaluation of the $I$'s. The results are tabulated in Table Ah-2 below.

<table>
<thead>
<tr>
<th>Integral</th>
<th>$\alpha = .1$</th>
<th>$\alpha = .15$</th>
<th>$\alpha = .2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$J_1$</td>
<td>.027</td>
<td>.040</td>
<td>.051</td>
</tr>
<tr>
<td>$J_1$</td>
<td>.013</td>
<td>.022</td>
<td>.031</td>
</tr>
<tr>
<td>$J_1 + J_2$</td>
<td>.040</td>
<td>.062</td>
<td>.082</td>
</tr>
</tbody>
</table>

Intermediate integrals in the evaluation of $\delta_{17}^{(2)}$ which gives the effect on the annihilation rates of electron hole-electron interactions (diagram 4-1c).
Appendix 5

Evaluation of Some Integrals Giving the Effect of Self Energies on the Angular Correlation Curve for $f^2 g^2$.

Integral 1.

From formula (5-8), the contribution to $\Theta_1^{(1)}$ from the electron self energy diagram 5-1b is

$$
\Theta_1^{(1)} = \frac{(\gamma_0^2 \lambda)}{V^2} \int \frac{d\epsilon}{2\pi} \bar{u}(q; \epsilon) \left( \frac{\epsilon}{(p-\epsilon)^2} + \frac{1}{(p-(q-q)^2+\epsilon i)^2} \right).
$$

Since there are no singularities of the integrand in (A5-1) in the first and third quadrants of the complex $\epsilon$-plane, the integration can be switched to one along the imaginary axis and its range restricted to $(0, \infty)$. Thus

$$
\Theta_1^{(1)} = \frac{(\gamma_0^2 \lambda)}{V^2} \int \frac{d\epsilon}{2\pi} \bar{u}(q; \epsilon) \left[ \frac{1}{(p-\epsilon)^2} + \frac{1}{(p-(q-q)^2+\epsilon i)^2} \right].
$$

To do the angular part of the $\theta$ integration in (A5-2), apply the rule (A2-3). This yields

$$
\Theta_1^{(1)} = \frac{\lambda}{V^2} \int_{\frac{\pi}{2}}^{\infty} d\epsilon \int_{\frac{\pi}{2}}^{\infty} \bar{u}(q; \epsilon) \left[ \frac{(p-\epsilon)^2}{[(p-\epsilon)^2+\epsilon^2]^2} \right].
$$
Using (A5-4) in (A5-3) gives

\[
R_{\xi}^{(ab)} = \frac{1}{V} \left[ \frac{1}{\tilde{Q}^2} \int_{0}^{\infty} d\epsilon \int_{0}^{\infty} \frac{dP_{\epsilon}}{P} \frac{dP_{\tilde{Q}}}{P_{\tilde{Q}}} \epsilon \left[ \frac{\epsilon^2 + \frac{1}{\tilde{Q}^2}}{\epsilon^2 + \frac{1}{P_{\tilde{Q}}^2}} \right] - \frac{\tilde{Q}^2}{P_{\tilde{Q}}^2} \frac{P_{\tilde{Q}}^2}{P_{\epsilon}^2} \right] .
\]

For the numerical evaluation of (A5-5), it is convenient to make the transformation \( \epsilon \to \frac{\epsilon}{P_F} \), then measure all momenta in units of \( P_F \), and send \( \epsilon \to \epsilon P_F \). Finally, introducing the parameter \( \xi \) yields

\[
R_{\xi P}^{(ab)} = \frac{1}{V} \left[ \int_{0}^{\infty} d\epsilon \int_{0}^{\infty} \frac{dP_{\epsilon}}{P} \frac{dP_{\xi}}{P_{\xi}} \epsilon \left( \frac{\epsilon^2 + \xi^2}{\epsilon^2 + \frac{1}{P_{\xi}^2}} \right) - \frac{\xi^2}{P_{\xi}^2} \frac{P_{\xi}^2}{P_{\epsilon}^2} \right] .
\]

The results of the numerical evaluation of (A5-6) are presented in Table A5-1.
Table A5-1

<table>
<thead>
<tr>
<th></th>
<th>$\gamma = 1$</th>
<th>$\gamma = 1.5$</th>
<th>$\gamma = 1.9$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\xi_{\alpha}(\infty)$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\xi_{\alpha}(\infty)$</td>
<td>$-0.00909$</td>
<td>$-0.01886$</td>
<td>$-0.07576$</td>
</tr>
<tr>
<td>$\xi_{\alpha}(\infty)$</td>
<td>$-0.1281$</td>
<td>$-0.06467$</td>
<td>$-0.17078$</td>
</tr>
</tbody>
</table>

Momentum dependence of $\xi_{\alpha}(\infty)$ which gives the effect of electron self energies of the partial annihilation rate. The variable $\gamma$ is momentum in units of $\frac{1}{c}$ and the parameter $\alpha$ is related to $\alpha_{s}$ by $\alpha = \alpha_{s}(1.11 \pi)$.

Integral 2.

For the positron self energy case, the integral that enters is from formula (5-16):

$$
\xi^{(ic)}_{\alpha} = \frac{i}{\sqrt{2}} \int_{0}^{\infty} \frac{d\xi}{2\pi} \left\{ \frac{\Theta(p_{-}, p_{+})}{(-\xi^{2} - \epsilon + i\gamma)^{2}} - \frac{\Theta(p_{-}, 1 + p_{+})}{(-\xi^{2} - \epsilon - i\gamma)^{2}} \right\}.
$$

(A5-7)

Again, a switch to the imaginary $\epsilon$-axis gives

$$
\xi^{(ic)}_{\alpha} = \frac{1}{\sqrt{2}} \int_{0}^{\infty} \frac{d\xi}{2\pi} \left\{ \frac{\Theta(p_{-}, p_{+})}{(-\xi^{2} + \epsilon^{2})^{2}} - \frac{\Theta(p_{-}, 1 + p_{+})}{(-\xi^{2} + \epsilon^{2})^{2}} \right\}.
$$

(A5-8)

To do the angular part of the $q_{\beta}$ integration in the second term of (A5-8), apply the rule
which can easily be verified using methods similar to those described in Appendix 2. Thus the second term becomes

\[ -\lambda \frac{1}{V (2\pi)^2} \int_{0}^{\infty} d^3 \mathbf{q} \int_{0}^{1} d\xi u(\xi) \frac{q^2}{q^2 + \xi^2} \frac{1}{(q^2 + \xi^2)^2} \]

\[ -\lambda \frac{1}{V (2\pi)^2} \int_{0}^{\infty} d^3 \mathbf{p} \int_{0}^{1} d\xi u(\xi) \frac{p^2 - (\xi - 1)^2}{(p^2 + \xi^2)^2} \]

Finally, making use of the same series of transformations on (A5-10) and on the first term of (A5-8) as were carried out on Integral 1 gives

\[ \Theta_{p_F, \nu}^{(0)} = \frac{\lambda}{V} \int_{0}^{1} d\alpha \int_{0}^{\infty} \frac{d\xi}{q^2 + \alpha \mathcal{Q}(q, \xi)} \frac{1}{(q^2 + \alpha \mathcal{Q}(q, \xi))^2} \]

\[ -\frac{\lambda}{V} \int_{0}^{1} d\alpha [1 - (\xi - 1)^2] \int_{0}^{\infty} \frac{d\xi}{q^2 + \alpha \mathcal{Q}(q, \xi)} \frac{q^2 - \xi^2}{(q^2 + \alpha \mathcal{Q}(q, \xi))^2} \]

To economize on computer time the numerical evaluation of this integral was carried out only for \( \alpha = 2 \). For the numerical results see Table A5-2.

<table>
<thead>
<tr>
<th>Table A5-2</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \overline{\mathcal{R}}_{\nu}^{(1)} )</td>
</tr>
<tr>
<td>( \tau )</td>
</tr>
<tr>
<td>( \overline{\mathcal{R}}_{\nu}^{(2)} )</td>
</tr>
<tr>
<td>( \tau )</td>
</tr>
</tbody>
</table>

Momentum dependence of \( \overline{\mathcal{R}}_{\nu}^{(1)} \), which gives the effect of positron self energies on the partial annihilation rate. The variable \( \nu \) is momentum in units of \( p_F \).
Appendix 6

Evaluation of Some Integrals

Integral 1.

Formula (6-2) gives the contribution to \( \Theta_f \) for \( p > p_f \) from the first order electron self energy diagram as

\[
\Theta_{f}^{(ab)} = \frac{i}{V^2} \int_0^{\infty} \frac{d\beta}{\beta^2} \, u(\beta; \epsilon) \left( \epsilon^2 \frac{p^2 - p_f^2}{(\epsilon^2 + p_f^2)^2} \right) \frac{-i \Theta(p - p_f \beta)}{[p^2 - (p - p_f \beta)^2 - \epsilon^2 \beta^2]^2},
\]

where use was made of equation \( (A5.4) \). Finally,

\[
\Theta_{f}^{(11)} = \frac{1}{V (4\pi)^2} \int \frac{d\epsilon}{\epsilon} \, u(\epsilon; \epsilon) \left( \frac{\epsilon^2 - p_f^2}{\epsilon^2 + (p_f^2)^2} \right) \frac{-i \Theta(p - p_f \beta)}{[\epsilon^2 + (p_f^2)^2] \epsilon^2 + (p_f^2)^2}. \]

To do the \( \beta \) integration, the rule that must be used is

\[
\int_{p_f}^{p_f + p_f} \frac{d\beta}{\beta} \rightarrow \int_{p_f}^{p_f + p_f} \frac{d\beta}{\beta} \int_{\epsilon - \frac{p_f^2}{\epsilon}}^{\epsilon + \frac{p_f^2}{\epsilon}} \frac{d\epsilon}{\epsilon} \left( \frac{\epsilon^2 - p_f^2}{\epsilon^2 + (p_f^2)^2} \right) \frac{-i \Theta(p - p_f \beta)}{[\epsilon^2 + (p_f^2)^2] \epsilon^2 + (p_f^2)^2}. \]

This rule has essentially been established in discussing Integral 4 of Appendix 4. Applying (A6-2) to \( \Theta_{f}^{(ab)} \) yields

\[
\Theta_{f}^{(11)} = \frac{1}{V (4\pi)^2} \int \frac{d\epsilon}{\epsilon} \, u(\epsilon; \epsilon) \left( \frac{\epsilon^2 - p_f^2}{\epsilon^2 + (p_f^2)^2} \right) \frac{-i \Theta(p - p_f \beta)}{[\epsilon^2 + (p_f^2)^2] \epsilon^2 + (p_f^2)^2}. \]

where use was made of equation \( (A5.4) \). Finally,
The numerical results for this double integral are given in Table A6-1 for two values of $\alpha$.

\begin{align}
\Theta_{\Gamma p}^{(1b)} &= \frac{\Delta}{V} \int_{\mu - \hbar}^{\mu + \hbar} \int_{0}^{\infty} \frac{d\epsilon}{\epsilon^{2} + \alpha \omega} \left[ \frac{1}{\epsilon^{2} + \frac{1}{\epsilon^{2} + \alpha \omega^{2}}} - \frac{1}{\epsilon^{2} + \frac{1}{\epsilon^{2} + \alpha \omega^{2}}} \right].
\end{align}

The numerical results for this double integral are given in Table A6-1 for two values of $\alpha$.

<table>
<thead>
<tr>
<th>$\gamma = \rho_{p}/p_{0}$</th>
<th>$\Theta_{\Gamma p}^{(1b)} (\alpha = 1)$</th>
<th>$\Theta_{\Gamma p}^{(1b)} (\alpha = 2)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.1</td>
<td>0.0507</td>
<td>0.1021</td>
</tr>
<tr>
<td>1.2</td>
<td>0.0266</td>
<td>0.0592</td>
</tr>
<tr>
<td>1.3</td>
<td>0.0151</td>
<td>0.0359</td>
</tr>
<tr>
<td>1.4</td>
<td>0.0086</td>
<td>0.0221</td>
</tr>
<tr>
<td>1.5</td>
<td>0.0057</td>
<td>0.0154</td>
</tr>
<tr>
<td>1.6</td>
<td>0.0035</td>
<td>0.0101</td>
</tr>
<tr>
<td>1.7</td>
<td>0.0023</td>
<td>0.0067</td>
</tr>
<tr>
<td>1.8</td>
<td>0.0015</td>
<td>0.0046</td>
</tr>
<tr>
<td>1.9</td>
<td>0.0011</td>
<td>0.0031</td>
</tr>
</tbody>
</table>

Variation with momentum $\gamma$ (in units of $p_{0}$) of $\Theta_{\Gamma p}$, which gives the effect of electron self energies on the partial annihilation rate for $\gamma > 1$. The parameter $\alpha$ equals $\mathcal{R}_{c}/(0.914\pi^{2})$. The only diagram included is 5-1b.

**Integral 2**

From formula (6-8) the contribution to $\Theta_{p}$ from the first order positron self energy effect is

\[ \Theta_{p}^{(1c)} = \frac{\Delta}{V} \left( \frac{\epsilon}{\epsilon + \hbar} \right)^{3} \int_{\hbar}^{\epsilon_{F}} \int_{\mu - \hbar}^{\mu + \hbar} \frac{d\epsilon}{\epsilon^{2} + \alpha \omega} \left( \frac{1}{\epsilon^{2} + \frac{1}{\epsilon^{2} + \alpha \omega^{2}}} - \frac{1}{\epsilon^{2} + \frac{1}{\epsilon^{2} + \alpha \omega^{2}}} \right) \]
Carrying out the same series of algebraic steps on (A6-5) as on (A6-1), we obtain

\[
\mathcal{F}^{(c)}_{b' z'} = \frac{4 \pi}{V^2} \int \frac{d\phi}{\pi} \left\langle 1 - (1 - \nu_1)^2 \right\rangle \int_{\nu_1}^{\infty} \frac{\mathcal{E}' \mathcal{E}'}{\mathcal{E}'^2 + \alpha \mathcal{E}^2} \left( \frac{\mathcal{E}_1^2}{\mathcal{E}_2^2} \right)^2.
\]  

Table A6-2 gives the results of the numerical evaluation of (A6-6).

<table>
<thead>
<tr>
<th>\nu = \phi/\rho_0</th>
<th>\bar{\mathcal{Q}}^{(v)}_{\nu \rho_0} \text{ (A6-1)}</th>
<th>\bar{\mathcal{Q}}^{(v)}_{\nu \rho_0} \text{ (A6-2)}</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.05</td>
<td>0.0819</td>
<td>0.1397</td>
</tr>
<tr>
<td>1.15</td>
<td>0.0463</td>
<td>0.0857</td>
</tr>
<tr>
<td>1.25</td>
<td>0.0274</td>
<td>0.0550</td>
</tr>
<tr>
<td>1.35</td>
<td>0.0166</td>
<td>0.0361</td>
</tr>
<tr>
<td>1.45</td>
<td>0.0102</td>
<td>0.0239</td>
</tr>
<tr>
<td>1.55</td>
<td>0.0064</td>
<td>0.0159</td>
</tr>
<tr>
<td>1.65</td>
<td>0.0040</td>
<td>0.0107</td>
</tr>
<tr>
<td>1.75</td>
<td>0.0025</td>
<td>0.0072</td>
</tr>
<tr>
<td>1.85</td>
<td>0.0016</td>
<td>0.0049</td>
</tr>
<tr>
<td>1.95</td>
<td>0.0010</td>
<td>0.0033</td>
</tr>
</tbody>
</table>

Variation with momentum \( \nu \) (in units of \( \rho_0 \)) of \( \bar{\mathcal{Q}}^{(v)}_{\nu \rho_0} \) which gives the effect of positron self energies on the partial annihilation rate for \( \nu > 1 \). The diagram included is 5-10.

Integral 3\nu

Formula (6-9) gives \( \mathcal{F}^{(i)}_{i'} \) from the first order ladder graph and can be rewritten in the form
\[ \mathcal{R}_{\gamma'}^{(\alpha)} = \frac{1}{V} \int \frac{d^3k}{(2\pi)^3} \int_0^\infty \frac{d\omega}{\omega} \frac{U(k,i\omega)}{k^2 + \omega^2} \frac{1}{k^2 + (k\cdot p_F)^2} \left[ k \frac{\omega^2 + (k\cdot p_F)^2}{(k^2 + \omega^2)^2} \right] \left[ \frac{\omega}{k^2 + \omega^2} \right] \left[ \tan^{-1} \left( \frac{k^2 - \omega^2}{2\omega} \right) \right] \]

The results from the numerical evaluation of this double integral are given in Table A6-3.

<table>
<thead>
<tr>
<th>( x' )</th>
<th>( \rho/\rho_s )</th>
<th>( \mathcal{R}_{\gamma'}^{(\alpha)} (\alpha = 1) )</th>
<th>( \mathcal{R}_{\gamma'}^{(\alpha)} (\alpha = 2) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.1</td>
<td>0.1074</td>
<td>0.2037</td>
<td></td>
</tr>
<tr>
<td>1.2</td>
<td>0.0595</td>
<td>0.1235</td>
<td></td>
</tr>
<tr>
<td>1.3</td>
<td>0.0359</td>
<td>0.0776</td>
<td></td>
</tr>
<tr>
<td>1.4</td>
<td>0.0211</td>
<td>0.0499</td>
<td></td>
</tr>
<tr>
<td>1.5</td>
<td>0.0135</td>
<td>0.0346</td>
<td></td>
</tr>
<tr>
<td>1.6</td>
<td>0.0085</td>
<td>0.0231</td>
<td></td>
</tr>
<tr>
<td>1.7</td>
<td>0.0055</td>
<td>0.0156</td>
<td></td>
</tr>
<tr>
<td>1.8</td>
<td>0.0036</td>
<td>0.0106</td>
<td></td>
</tr>
<tr>
<td>1.9</td>
<td>0.0024</td>
<td>0.0073</td>
<td></td>
</tr>
</tbody>
</table>

Variation with momentum \( x' \) (in units of \( \rho_s \)) of \( \mathcal{R}_{\gamma'}^{(\alpha)} \), which gives the effect of the first order ladder graph 5-1a on the partial annihilation rate for \( x' > 1 \).
Sum of Integrals 1, 2, and 3

The numerical work on \( \widehat{\mathbf{B}}_{1,2}^{\text{th}} \) was done quite roughly and is probably good to only 1 or at most 2 figures. But when integrals 1, 2 and 3 are summed, their first two significant figures cancel (approximately). Hence to get a meaningful number for the sum it was necessary to re-evaluate \( \widehat{\mathbf{B}}_{1,2}^{\text{th}} \) as a single integral. The work was carried out only for \( \alpha = 0.2 \) and the results are shown in Table A6-4. The cancellation is almost complete, i.e. \( \widehat{\mathbf{B}}_{1,2}^{\text{th}} \) is almost as large (but negative) as the sum of \( \widehat{\mathbf{B}}_{1,2}^{\text{th}} \) and \( \widehat{\mathbf{B}}_{1,2}^{\text{th}} \).

Table A6-4

<table>
<thead>
<tr>
<th>( \gamma )</th>
<th>1.1</th>
<th>1.3</th>
<th>1.5</th>
<th>1.7</th>
<th>1.9</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \widehat{\mathbf{B}}_{1,2}^{\text{th}} )</td>
<td>.0075</td>
<td>.0030</td>
<td>.0014</td>
<td>.0007</td>
<td>.0003</td>
</tr>
</tbody>
</table>

Sum of \( \widehat{\mathbf{B}}_{1,2}^{\text{th}} + \widehat{\mathbf{B}}_{1,2}^{\text{th}} + \widehat{\mathbf{B}}_{1,2}^{\text{th}} \) for \( \alpha = 0.2 \).

Monte Carlo integrals.

There are three integrals to be evaluated by a Monte-Carlo method. These are integrals (6-7), (6-10), and (6-11). If in integral (6-7) the coulomb potential functions \( \Psi_{\pm} \) and \( \Psi_{\pm}^\prime \) are replaced by the static screened coulomb potential, \( \Phi_{e}^{(\text{sd})} \), then the potential becomes

\[
\Phi_{e}^{(\text{sd})} = -\frac{1}{\sqrt{\Gamma}} \int d\gamma \Psi_{\pm}^{*} \Psi_{\pm}^\prime \frac{\Theta(p+q+\xi-a_{p}) \Theta(p-\xi) \Theta(p-\xi+q')}{[p^2+(q+\xi)^2 -(q+\xi-a_{p})^2 -(q+\xi+a_{p})^2]^2}. \tag{A6-7}
\]

Make the following transformations on (A6-9): send \( q \rightarrow -k \) and \( q+q' \rightarrow -k' \); then measure all momenta in units of \( p_{F} \) and introduce the parameter \( \alpha = 1/(\sqrt{2}p_{F}^2) \). This gives

\[
\Phi_{e}^{(\text{sd})} = -\alpha^2 \int_{-k}^{+k} \int_{-k}^{+k} \frac{U(p+q+k)U(p+q+k')}{[(q^2-k^2-k'^2)^2 +(q+q'+k)^2]^2}. \tag{A6-10}
\]
The variation with momentum ( \( \nu \) in units of \( p_f \) for \( \nu > 1 \) ) of \( \delta \rho \) and \( \delta \rho' \), which give the effect of particle-hole interactions on \( \Theta \). Also shown is \( \Theta_{\nu} \), as a function of \( \nu \), which gives the correction to the electron momentum distribution from the exchange self energy diagram 6-14.  

where \( \Omega(t) \) is as given in formula (4-16). In this form (6-10) can readily be evaluated by Monte-Carlo integration methods. The computer program used was almost identical to the one described in reference . The other two integrals of interest differ from (6-7) only in the integrand. The restrictions on the range of integration are the same. By a series of transformations similar to those carried out on \( \Theta_c(\nu) \), \( \Theta_{\nu} \) and \( \Theta_{\nu'} \), given by
(6-10) and (6-11) respectively can indeed be written as

\[ \Theta_{e^- e^-} > = -\frac{\lambda e^2}{\nu} \int_{k' < 1} d^3 k' \int_{k < 1} d^3 k \left[ \frac{U(1k + k') U(1k' + k')}{(k' + k + y)^2 - (k + k + y)^2} \right] \]

and

\[ \Theta_{e^- e^-} > = \frac{\lambda e^2}{\nu} \int_{k' < 1} d^3 k' \int_{k < 1} d^3 k \left[ \frac{U(1k + k') U(1k' + k')}{(k' + k + y)^2 - (k + k + y)^2} \right] \]

The results of the computer program are given in Table 46-5.

The numerical evaluation of \( \Theta_7a \) + \( \Theta_7b \) + \( \Theta_7c \) in the Born approximation.

The electron part of (6-42) can be written as

\[ \Theta_7^{(e)} = \frac{2\pi i}{\nu^2} \int \frac{d\nu}{2\pi} \frac{\nu(1\nu - \nu - 1\nu - 1\nu - 1\nu)}{[\nu(1\nu - \nu - 1\nu - 1\nu - 1\nu)]^2} \chi_0^0 (\nu + \nu + \nu - \nu - \nu - \nu) \]

The angular integration in (A6-11) can be carried out by using methods similar to those used on (A6-1). The manipulations are too tedious to give here, but our final result is
\[ \Theta_2^{(0)} = \frac{1}{\sqrt{3}} \left( \frac{\pi}{2} \right) \int_0^{\pi} \frac{d\phi}{\gamma(\phi)} \left[ \frac{1}{\sqrt{2}} \int_0^{\alpha} d\alpha \left( \frac{1}{(1-\alpha^2)^2} \right) \right] \]

\[ q_1(1-\alpha^2) \times \left[ \frac{q^2 - q'^2}{2} \right] I_2(p, q, \alpha) - [ (p - q)^2 \alpha^2 - (1-\alpha^2)^2 I_1(p, q, \alpha) ] \]  \tag{A6-12}

with

\[ I_1(p, q, \alpha) = \int_0^{\pi} \frac{d\alpha}{q^2 + \alpha^2} \left[ \tan^{-1} \left( \frac{\alpha}{p} \right) \right] \]

\[ + \int_0^{\pi} \frac{d\alpha}{q^2 + \alpha^2} \left[ \tan^{-1} \left( \frac{\alpha}{1+q} \right) \right] \]

\[ + \int_0^{\pi} \frac{d\alpha}{q^2 + \alpha^2} \left[ \tan^{-1} \left( \frac{\alpha}{1-q} \right) \right] \]

\[ \Theta_2^{(2)} = \frac{e^{i\pi}}{2\alpha} \left[ 1 - \frac{1}{2} \left[ 1 - \frac{1}{2} (1-\alpha^2)^2 \right] \ln \left( \frac{(1-\alpha^2)^2}{(1-\alpha^2)^2 (2\alpha^2 - 2\alpha^2)} \right) \right] \]

\[ + \frac{(1-\alpha^2)}{2\alpha} \left[ \tan^{-1} \left( \frac{\alpha (2\alpha - 1)}{1-\alpha^2} \right) + \tan^{-1} \left( \frac{\alpha (2\alpha + 1)}{1-\alpha^2} \right) \right] \]

and

\[ \Theta_2 = \frac{1}{2\kappa} \left[ 1 + \frac{1}{2\kappa} \left( 1 + \kappa^2 \right) \right] \ln \left\{ \frac{\alpha^2 \kappa^2}{\alpha^2 \kappa^2 (2\alpha^2 - 2\alpha^2)} \right\} \]

All \( \psi \)'s on the right hand side of (A6-12) are to be read as \( \psi \)'s.
The polarization part of (6-52) can be dealt with in the same way. The numerical work on $\Theta_{f}^{1a}$ and $\Theta_{f}^{1b}$ was carried out on the Toronto IBM 7090 computer for $\alpha = 0.211$, i.e. $\alpha^2 \geq 4$, and 5 values of momentum $p > p_{f}$. The results are given in Table A6-6.

**Table A6-6**

<table>
<thead>
<tr>
<th>$\tau$</th>
<th>$\Theta_{f}^{1a}$</th>
<th>$\Theta_{f}^{1b}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.1</td>
<td>-0.2140</td>
<td>0.2106</td>
</tr>
<tr>
<td>1.3</td>
<td>-0.0773</td>
<td>0.0704</td>
</tr>
<tr>
<td>1.5</td>
<td>-0.0320</td>
<td>0.0277</td>
</tr>
<tr>
<td>1.7</td>
<td>-0.0140</td>
<td>0.0118</td>
</tr>
<tr>
<td>1.9</td>
<td>-0.0064</td>
<td>0.0053</td>
</tr>
</tbody>
</table>

$\Theta_{f}^{1a}$ and $\Theta_{f}^{1b}$ as functions of momentum $\tau$ for $\tau > 1$. These values apply to the case $\alpha^2 \geq 4$. 
REFERENCES

   (Referred to in this thesis as LW-I)
   (Referred to in this thesis as K-I.)
   (Referred to in this thesis as K-II)
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