THERMALIZATION TIME OF POSITRONS IN METALS

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By

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ABSTRACT:

The thermalization time of positrons in metals has been computed as a function of the electron density parameter r_s, in the complete metallic electron density range ($2 < r_s < 5.6$). Our calculations are based on the propagator technique of many-body perturbation theory, to first order in the electron-positron effective force. The rate of energy loss of the positron, in our formalism, is given by the imaginary part of the self energy operator; this quantity is worked out both in the Random Phase and the Hubbard approximation. We find that, in the low momentum transfer region, which is really the only regime of importance here, the electron-positron interaction can be approximated by a screened Coulomb potential $\frac{e^2}{r} \exp(-\lambda_{TF} r)$ where λ_{TF} is the

Thomas-Fermi momentum given by $\sqrt{4\pi\alpha}\ p_F$. Here α is related to r_s, the usual density parameter, by $\alpha = \frac{r_s}{1.919\pi^2}$.

Further, we find that, in general, the time taken by the positron to drop to an energy of .025 e.v. is not as short as is generally believed, although it can be said beyond doubt that complete thermalization has taken place before annihilation at room temperature. However, for aluminium at $100^{\circ}k$, the thermalization time is <u>longer</u> than the annihilation time. On the basis of this result, we suggest that this lack of thermalization in aluminium might be detectable in an experiment similar to that recently reported by Stewart and Shand (1966), concerning the positron effective mass in sodium, although without more extensive calculations it is not possible to say <u>precisely</u> how a small amount of non-thermalization would affect the angular correlation curves.

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CHAPTER I

Introduction

The thermalization time of a positron in a metal is the interval of time between the instant a relatively high energy positron enters into the metal and that at which it achieves thermal equilibrium with the conduction electron gas. A knowledge of this characteristic time τ_T is pertinent to the interpretation of the experimental angular correlation data and the total annihilation rate. It is usually taken for granted that the positron is thermalized before annihilation. While a small amount of non-thermalization would not change the shape of the (overall) angular correlation curves very much, the recent experiments on the positron motion in sodium reported by Stewart and Shand (1966), however, depend quite critically for their interpretation and consequently, for their conclusions, on the assumption that the positron is thermalized prior to annihilation. Thus, the determination of the thermalization time, by a detailed analysis, is an illuminating problem.

Apart from these reasons, from a theoretical point of view, a study of the entity τ_T is interesting in its own right. It provides an insight into the various polarization processes occurring in the medium such as the creation of electron hole-particle pairs and the back influence of the resulting polarization charge on the positron and, consequently, on the rate at which it loses energy.

It seems that not much work has been reported on the calculation of τ_T even after the advances in many-body theory. The recent experimental attempt to determine τ_T directly, (Stewart & Shand (196 on the other hand, does not yet appear to have reached the accuracy needed. Lee-Whiting's (1955) theoretical calculations of τ_T is the only published work, available to date. This work was done before many-body techniques were well established.

Lee-Whiting represents the interaction between a positron and a polarizable free-electron gas by a screened Coulomb potential of the form $\frac{e^2}{r} \exp(-\lambda r)$, where e is the electronic charge, r is the relative distance between the positron and an electron and λ is the screening parameter. The parameter λ is, to some extent, arbitrary and to be fixed in a reasonable way. It is further assumed that the value of λ appropriate for positron-electron interaction is the same as that suitable for electron-electron interaction. The Exclusion Principle does not

apply to the electron-positron system. The initial state of the system is taken to be a free electron gas with a polarization cloud about each electron. It is further assumed that, in this model, the positron interacts with free electrons through a screened Coulomb interaction. The positron being in a high energy level, is then capable of losing energy to the medium by creating real electron hole-particle pairs. Thus it loses its energy to the medium continuously and tends towards thermal equilibrium with the electron gas. The rate of energy loss is a function of the positron energy and is extremely sensitive to the parameter λ. In fact $R \propto \lambda^{-4}$.

Basing his argument on the available experimental data in related fields and the theoretical situation at that time, Lee-Whiting took $\lambda = 1.02 \times 10^{8}$ cm^{-1} for sodium. Thus τ_T for sodium was found to be 3×10^{-12} sec., whereas the annihilation time $\tau_A = 3.4 \times 10^{-10}$ sec., so that $\frac{\tau_A}{\tau_T} = 113$. Hence, according to Lee-Whiting, a positron is certainly thermalized before annihilation.

Our approach to the problem is on a similar line of physical argument to Lee-Whiting's. However, in the light of advances in many-body theory, we propose, in this work, to tackle the problem in a somewhat more fundamental way, by using the Green's function propagator technique of the many-body perturbation theory. We will consider only the first order effects, assuming

that the higher order contributions are negligible in comparsion. Nevertheless, the dynamic dielectric function will be used in determining the effective potential.

In Chapter 2, the theory will be developed by using the propagator technique and an expression will be found for the irreducible self energy operator $M(\underset{\sim}{k};\ \omega)$ in the Random Phase Approximation (R.P.A.). An expression for the rate of energy loss $R[\underset{\sim}{k}]$ of the positron as a function of its momentum $\underset{\sim}{k}$ will be obtained in Chapter 3. This expression is obtained quite directly from the imaginary part of the self energy operator $M(\underset{\sim}{k};\ \omega)$. Chapter 4 is merely concerned with the algebraic reduction of the expression for $R[\underset{\sim}{k}]$ to be ready for computation. Also the real and imaginary parts of the dynamic dielectric function, in the R.P.A., will be computed and compared, in the low energy and momentum transfer range, with the static limit.

The formalism of Chapter 2 will be extended in Chapter 5 to take account of the Hubbard correction to the R.P.A., which can be important at metallic densities.

Finally, in Chapter 6, we discuss the results obtained and draw conclusions. In the end, we propose an experiment in aluminium similar to that reported by Stewart and Shand in sodium, which might be expected to show effects of lack of positron thermalization.

CHAPTER 2

The Positron Propagator

Let us consider a positron propagating through a metal. We neglect the lattice entirely, replacing it by a fixed background of positive charge neutralizing the system. The positron Green's function $G_p(x;\ x')$, which can then depend only on the relative space and time coordinates, is defined by

$$G_p(x;\ x') = i \langle N \mid T\ \phi(x)\ \phi^+(x') \mid N \rangle \qquad (2.1)$$

where $|N\rangle$ is the fully interacting Heisenberg ground state for the N conduction electrons, and T is the Wick's time ordering operator (1950). $\phi^+(x)$ and $\phi(x)$ are respectively the particle creation and destruction operators for the positron field in the Heisenberg picture. Notice that for $t' > t$, $G_p(x;\ x')$ vanishes. To start with, we consider the system to be noninteracting. We will, later on, account for interactions by perturbation theory. In this approximation, equation (2.1) becomes

$$G_p^o(x;\ x') = \frac{i}{V} \sum_{\underset{\sim}{k}} e^{\left[i \underset{\sim}{k}\cdot(\underset{\sim}{x}-\underset{\sim}{x}') - i k^2 (t-t')\right]} \qquad \text{for } t > t'$$

$$= 0 \qquad \text{for } t' > t \qquad (2.2)$$

where $\underset{\sim}{k}$ is the positron momentum and V is the volume of the metal; also we have taken units such that $2m = \hbar = 1$.

By space and time Fourier transforming, (2.2) becomes

$$G_p^o(\underset{\sim}{k};\ \omega) = \frac{1}{k^2-\omega-io^+}, \tag{2.3}$$

where all Fourier transforms are defined by

$$F(x;\ x') = \frac{1}{V} \sum_{\underset{\sim}{k}} e^{i\underset{\sim}{k}\cdot(\underset{\sim}{x}-\underset{\sim}{x}')} \int \frac{d\omega}{2\pi} e^{-i\omega(t-t')} \times F(\underset{\sim}{k};\ \omega) \tag{2.4}$$

The positron Green's function (propagator) for the interacting system is related to the noninteracting propagator by the well-known Dyson equation:

$$G_p(\underset{\sim}{k};\ \omega) = G_p^o(\underset{\sim}{k};\ \omega) + G_p^o(\underset{\sim}{k};\ \omega)\ M(\underset{\sim}{k};\ \omega)\ G_p(\underset{\sim}{k};\ \omega) \tag{2.5}$$

where $M(\underset{\sim}{k};\ \omega)$ is the irreducible self-energy operator.

We are concerned, in this work, with the determination of the thermalization time. This can be easily calculated from

the rate of energy loss of the positron. And it will be shown in Chapter 3, that the rate of energy loss is, in turn, directly related to the imaginary part of the irreducible self-energy operator $M(\underset{\sim}{k};\ \omega)$ (Dubois (1959)). Hence it is more appropriate to approximate directly to the operator $M(\underset{\sim}{k};\ \omega)$ rather than to the Green's function $G_p(\underset{\sim}{k};\ \omega)$.

Going back to the Dyson equation (2.5) (which is just a linear equation), its solution is given by

$$G_p(\underset{\sim}{k};\ \omega) = \frac{G_p^o(\underset{\sim}{k};\ \omega)}{1-G_p^o(\underset{\sim}{k};\ \omega)\, M(\underset{\sim}{k};\ \omega)},$$

and making use of (2.3), we have

$$G_p(\underset{\sim}{k};\ \omega) = \frac{1}{k^2 - \omega - M(\underset{\sim}{k};\ \omega)} \tag{2.6}$$

Equation (2.6) is an exact equation of motion of the positron in the medium; $M(\underset{\sim}{k};\ \omega)$ accounts for interactions. When it vanishes, we recover, of course, the noninteracting propagator. It should be clear now from the explicit form of G in (2.6) that it is more convenient to work with M rather than G, since M represents a direct correction to the noninteracting motion of the positron. In particular, its imaginary part gives the damping of the positron motion.

To begin with, we shall treat $M(x;\ x')$ in the Random Phase Approximation, which means that we will include in our calculation only those graphs which are shown in Figure (1a). In Chapter 5, however, we shall correct the R.P.A. formulation by including the interactions between the created electron hole-particle pairs, as first suggested by Hubbard (1957). It is enough to remark here, however, that in our region of interest, Hubbard corrections do not modify our results significantly and that the R.P.A. is a good approximation.

Obviously, the first graph in this infinite series has no contribution, since it involves the time ordering $t' - t > 0$ (with $(t'-t) \longrightarrow 0$) of the propagator $G_p(x;\ x')$ which, from equation (2.2), is zero. In any case, this is the first member of the infinite set of Feynman's graphs of interest here and, therefore, we will include it for the sake of continuity argument. Finally, this infinite set of graphs is written identically equal to the graph (1b) by introducing the effective potential $\mu(x;\ x')$.

The integral equation representing $\mu(x;\ x')$ is shown diagrammatically in Figure 2. Mathematically,

$$\mu(x;\ x') = V(x;\ x') - i \int V(x;\ z)\, Q^{RPA}(z;\ z')\, \mu(z';\ x')\, d^4z\, d^4z'$$

where Q^{RPA} is the polarization part in R.P.A. and V is the bare coulomb potential.

Taking space-time Fourier transforms, it reads

$$\mu(\underset{\sim}{q};\ \epsilon) = V_{\underset{\sim}{q}} - 2\, V_{\underset{\sim}{q}}\, Q^{RPA}(\underset{\sim}{q};\ \epsilon)\ \mu(\underset{\sim}{q};\ \epsilon) \qquad (2.7)$$

Here $V_{\underset{\sim}{q}} = \dfrac{4\pi e^2}{q^2}$ where e is the electronic charge. The factor of 2 is included for spin degeneracy.

The momentum frequency dependent polarization part in R.P.A. is defined in terms of the free electron propagator $G_e^o(\underset{\sim}{k};\ \omega)$ as

$$Q^{RPA}(\underset{\sim}{q};\ \epsilon) = \frac{i}{V} \sum_{\underset{\sim}{k}} \int \frac{d\omega}{2\pi}\, G_e^o(\underset{\sim}{k}+\underset{\sim}{q};\ \omega+\epsilon) \times G_e^o(\underset{\sim}{k};\ \omega)$$

$$= -\frac{1}{V} \sum_{\underset{\sim}{k}} \left[\frac{\theta(k-P_F)\,\theta(P_F-|\underset{\sim}{k}+\underset{\sim}{q}|)}{(\underset{\sim}{k}+\underset{\sim}{q})^2 - k^2 - \epsilon + io^+} - \frac{\theta(P_F-k)\,\theta(|\underset{\sim}{k}+\underset{\sim}{q}|-P_F)}{(\underset{\sim}{k}+\underset{\sim}{q})^2 - k^2 - \epsilon - io^+} \right] \qquad (2.8)$$

where θ's are step functions; for example,

$$\theta(k - P_F) = 1 \quad \text{for } k > P_F$$
$$= 0 \quad \text{for } k < P_F$$

Here P_F = Fermi momentum.

Solving equation (2.7) for the effective potential, we have

$$\mu(\underset{\sim}{q};\ \epsilon) = \frac{V_q}{1 + 2\, V_{\underset{\sim}{q}}\, Q^{RPA}(\underset{\sim}{q};\ \epsilon)} \qquad (2.9)$$

$$= \frac{V_q}{\epsilon(\underset{\sim}{q};\ \epsilon)}$$

where $\epsilon(q;\ \epsilon)$ is the dynamic dielectric function for the electron medium. A knowledge of the dielectric function is pertinent to our problem. Because of the direct relationship between Q and ϵ,

$$Q = \frac{\epsilon - 1}{2\, V_{\underset{\sim}{q}}} ,$$

we shall investigate the behaviour of the polarization operator Q, in detail.

As shown in Figure (1b), the self-energy operator M can be written in terms of the effective potential as

$$M(x;\ x') = i\, G_p^o(x;\ x')\ \mu(x;\ x') \qquad (2.10)$$

The physical interpretation of this equation, which gives an

insight into the actual processes taking place, is as follows. The positron creates an electron hole-particle excitation in a fully interacting medium. The excitation and the positron then propagate independently for some time before the excitation interacts back on the positron affecting its trajectory. It is this screened coulomb force, including the virtual polarization of the medium which determines its rate of energy loss and, consequently its thermalization time.

Notice that we are considering the first order effects only in the electron-positron coupling, assuming that the second and higher-order effects can be neglected, in comparison to this.

Fourier transforming (2.10), one obtains

$$M(\underset{\sim}{k};\ \omega) = \frac{i}{V} \sum_{\underset{\sim}{q}} \int \frac{d\epsilon}{2\pi}\ \mu(\underset{\sim}{q};\ \epsilon)\ G_p^o\ (\underset{\sim}{k}-\underset{\sim}{q};\ \omega-\epsilon) \tag{2.11}$$

$$= \frac{i}{V} \sum_{\underset{\sim}{q}} \int \frac{d\epsilon}{2\pi}\ \mu\ (\underset{\sim}{q};\ \epsilon)\ \frac{1}{(\underset{\sim}{k}-\underset{\sim}{q})^2 - \omega + \epsilon - i0^+}$$

where we have made use of (2.3).

The analytic properties of the integrand in (2.11) as a function of the complex variable ϵ consist of the singularities

of $\mu(\underset{\sim}{q};\ \epsilon)$ plus the extra pole of $\epsilon = \omega - (\underset{\sim}{k}-\underset{\sim}{q})^2 + io^+$. The ϵ-integral has been worked out by Carbotte (1964) and the result is

$$M(\underset{\sim}{k};\ \omega) = \frac{2}{V^2} \sum_{\underset{\sim}{q}\underset{\sim}{q}'} \frac{\theta(P_F-q')\ \theta(|\underset{\sim}{q}' - \underset{\sim}{q}| - P_F)\ V_q^{\,2}}{\left| 1 + 2\, V_{\underset{\sim}{q}}\, Q^{RPA}(\underset{\sim}{q};\ (\underset{\sim}{q}'-\underset{\sim}{q})^2 - q'^2 \right|^2}$$

$$\times \frac{1}{(\underset{\sim}{k}-\underset{\sim}{q})^2 - \omega + (\underset{\sim}{q}' - \underset{\sim}{q})^2 - q'^2 - io^+} \qquad (2.12)$$

We have dropped the contribution to M from the plasmon pole, since we are interested only in a formula for the rate of energy loss in the case of a low energy positron, i.e., having an energy of say 5 e.v. or less. Plasmon energies are, in general, considerably higher than this so that, in the region of interest here, plasmon creation is not a possible mechanism of energy transfer.

As a function of complex ω, the singularities of $M(\underset{\sim}{k};\ \omega)$ can be easily read from the expression (2.12). It has a cut extending from zero to infinity just below the real axis. This contribution comes from the continuum which implies the excitation of individual particles as opposed to collective

excitations like a plasma oscillation. $M(\underset{\sim}{k};\ \omega)$ has no singularities in the upper half plane. We shall make use of these properties of $M(\underset{\sim}{k};\ \omega)$ in the following chapter, where the actual positron propagator G_p will be shown to be very simply related to the imaginary part of the irreducible self-energy operator $M(\underset{\sim}{k};\ \omega)$.

CHAPTER 3

Formula for the Rate of Energy Loss

We shall now work out the expression for the rate of energy loss of the positron as a function of its momentum. For this purpose, we will be interested in the momentum time dependent positron propagator. Therefore, taking the Fourier transform of the positron Green's function from the frequency to the time plane, we have

$$G_p(\underset{\sim}{k};\ \tau) = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi}\ e^{-i\omega\tau}\ \frac{1}{k^2 - \omega - M(\underset{\sim}{k};\ \omega)} \tag{3.1}$$

where we have substituted from (2.6) into the prescription for the Fourier transform,

$$G_p(\underset{\sim}{k};\ \tau) = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi}\ e^{-i\omega\tau}\ G_p(\underset{\sim}{k};\ \omega) \tag{3.2}$$

The integral (3.1) can be worked out from our knowledge of the singularities of $M(\underset{\sim}{k};\ \omega)$ for complex ω. Provided that no new pole is introduced because of the appearance of the self-energy operator in the denominator, it is clear that $G_p(\underset{\sim}{k};\ \omega)$ has the same singularities as those of $M(\underset{\sim}{k};\ \omega)$. Now as a function of ω, $M(\underset{\sim}{k};\ \omega)$ has a cut extending from 0 to ∞ just below the real axis (coming from the continuum); the plasmon pole would introduce a further cut in part of this range, although this contribution has been omitted. Hence $M(\underset{\sim}{k};\ \omega)$ and therefore $G_p(\underset{\sim}{k};\ \omega)$ are both analytic in the upper half plane. Thus, $G_p(k;\ \infty)$ is zero for $\tau < 0$, since we can then close the contour in the upper half plane. This result is consistent with (2.2). Consider the case of $\tau > 0$. Close the contour below the real axis in the complex ω-plane.

As $e^{-i\omega\tau}$ damps out to zero on the contour γ (Figure 3(a)), therefore the contribution to the integral comes from the contour γ' (Figure 3(b)), which encloses the branch cut. Push the real axis down so that it coincides with the cut.

Then the closed integral

$$\oint_{\gamma} \frac{d\omega}{2\pi}\ e^{-i\omega\tau}\ f(\omega)$$

$$= \int_{\gamma'} \frac{d\omega}{2\pi}\ e^{-i\omega\tau}\ f(\omega)$$

$$= \int_0^{\infty} \frac{dx}{2\pi} \; e^{-ix\tau} \; f(x + io^+) + \int_{-\infty}^{0} \frac{dx}{2\pi} \; e^{-ix\tau} \; f(x - io^+)$$

$$= \int_0^{\infty} \frac{dx}{2\pi} \; e^{-ix\tau} \; (f(x + io^+) - f(x - io^+)) \qquad (3.3)$$

From eq. (3.1), since $M(\underset{\sim}{k}; \omega)$ has no imaginary part on the negative side of the real ω-axis, $G_p(\underset{\sim}{k}; \omega)$ is real for real $\omega < 0$. Therefore, by using the Schwartz reflection principle $f(\omega^*) = f^*(\omega)$, we can write

$$\lim_{\varepsilon \to 0^+} [f(x + i\varepsilon) - f(x - i\varepsilon)] = 2i \; \mathrm{Im} \; f(x) \qquad (3.4)$$

Hence the integral reduces to

$$\int_0^{\infty} \frac{dx}{2\pi} \; e^{-ix\tau} \; (2i) \; \mathrm{Im} f(x) \qquad (3.5)$$

In our problem

$$f(x \pm io^+) = \frac{1}{k^2 - x - E(\underset{\sim}{k}; \; x) \pm i/2 \; \Gamma(\underset{\sim}{k}; \; x)}$$

Since

$$M(\underset{\sim}{k};\ x \pm i\varepsilon^{+}) = E(\underset{\sim}{k};\ x) \pm \frac{i}{2}\ \Gamma\ (\underset{\sim}{k};\ x) \qquad (3.6)$$

Therefore

$$\text{Im } f(x) = \frac{\frac{1}{2}\ \Gamma\ (\underset{\sim}{k};\ x)}{< k^2 - x - E(\underset{\sim}{k};\ x) >^2 + \frac{1}{4}\ \Gamma^2(\underset{\sim}{k};\ x)} \qquad (3.7)$$

Thus equation (3.2) reduces to

$$G_p(\underset{\sim}{k};\ \tau) = \int_0^{\infty} \frac{dx}{2\pi}\ e^{-ix\tau}\ \frac{(2i)\ \frac{1}{2}\ \Gamma\ (\underset{\sim}{k};\ x)}{<k^2 - x - E(\underset{\sim}{k};\ x)>^2 + \frac{1}{4}\ \Gamma^2(\underset{\sim}{k};\ x)}$$

$$= \int_0^{\infty} \frac{dx}{2\pi}\ \frac{e^{-ix\tau}\ (i)\ \Gamma\ (\underset{\sim}{k};\ x)}{<k^2 - x - E(\underset{\sim}{k};\ x)>^2 + \frac{1}{4}\ \Gamma^2(\underset{\sim}{k};\ x)} \qquad (3.8)$$

The factor of $\frac{1}{2}$ in the imaginary part Γ of M has been taken for the sake of convenience in the following calculations.

Using the relation

$$\lim_{\varepsilon \to 0^{+}} \frac{1}{x - x_0 \pm i\varepsilon} = PP\ \frac{1}{x - x_0} \mp i\pi\delta\ (x - x_0),$$

the imaginary part of $M(\underset{\sim}{k};\ x)$ can be easily obtained from equation (2.12) and is given by

$$\frac{1}{2}\Gamma'(\underset{\sim}{k};\ x) = \frac{2}{V^2}\sum_{\underset{\sim}{q}\underset{\sim}{q}'} \frac{\theta(P_F - q')\,\theta(|\underset{\sim}{q}'-\underset{\sim}{q}| - P_F)\,V_q^{\,2}}{\left|1+2\,V_{\underset{\sim}{q}}\,Q^{RPA}(\underset{\sim}{q};\ (\underset{\sim}{q}'-\underset{\sim}{q})^2 - q'^2)\right|^2}$$

$$\times\,\pi\,\delta\left[(\underset{\sim}{k}-\underset{\sim}{q})^2 - x + (\underset{\sim}{q}'-\underset{\sim}{q})^2 - q'^2\right] \qquad (3.9)$$

The motion of the positron is damped by the induced hole-particle pairs and the extent of damping will be shown to be directly related to the imaginary part of $M(\underset{\sim}{k};\ x)$.

The integral (3.8) is easily evaluated for $\Gamma' \tau \ll 1$. For the perturbation theory to be valid, the quasi-particle energy shift as well as the damping rate should be small so that the integrand without the exponential in (3.8) is peaked at $x = k^2 - E(\underset{\sim}{k};\ x) \cong k^2$. The peak width is Γ'. Thus, provided the width is small as compared to the energy, which is the case in fact, we can extend the lower limit to $-\infty$ without making any change in the value of the integral. Therefore, the domain of integration can be taken to be $\in (-\infty, +\infty)$. The peak width Γ as a function of the positron energy for values of r_s (2 to 6) is worked out in the Appendix B and recorded in Table 1.

Now due to the presence of the oscillatory function $e^{-ix\tau}$, the peak is not so well defined. In order that the peak does not get chopped off due to oscillations, we assume that the wavelength of oscillations is much larger than the width of the peak so that the oscillatory function can be considered to be almost constant as x ranges over the Lorentzian (Figure 3c). Thus for $\Gamma\tau \ll 1$, we have, on replacing x by k^2 in $\Gamma(k;\ x)$,

$$G_p(\underset{\sim}{k};\ \tau) = \int_{-\infty}^{+\infty} \frac{dx}{2\pi} \quad \frac{(i)\, e^{-ix\tau}\, \Gamma(k;\ k^2)}{(x-k^2)^2 + \langle \tfrac{1}{2}\Gamma(\underset{\sim}{k};\ k^2)\rangle^2} \tag{3.10}$$

In order to evaluate this, let us consider the integral in the complex z-plane

$$\int_{-\infty}^{+\infty} \frac{dz}{2\pi} \quad \frac{e^{-iz\tau}}{(z-k^2)^2 + (\frac{1}{2}\Gamma)^2}$$

The integrand has poles at

$$z = k^2 - \frac{i}{2}\Gamma \quad \text{and} \quad z = k^2 + \frac{i}{2}\Gamma\ .$$

Now, for $\tau > 0$, the exponential dies out along the circle of radius $R \to \infty$, in the lower half plane. Therefore, we may close the contour below. Thus, closing the contour below, the residue of the function at the pole $k^2 - \frac{i}{2}\Gamma$ is

$$\frac{e^{-i(k^2 - \frac{i}{2}\Gamma)\tau}(-1)}{2\pi(-i\Gamma)}$$

The minus sign in the numerator appears because the contour has been taken in the clock-wise direction.

Hence

$$\int_{-\infty}^{+\infty} \frac{dx}{2\pi} \quad \frac{(i)\, e^{-ix\tau}\Gamma}{(x-k^2)^2 + \frac{\Gamma^2}{4}} = \frac{2\pi i}{2\pi i} \quad \frac{(i)\Gamma}{\Gamma} \quad x$$

$$\exp -i\,(k^2 - \tfrac{i}{2}\,\Gamma)\,\tau \qquad (3.11)$$

$$= (i)\, \exp \; -i\,(k^2 - \tfrac{i}{2}\,\Gamma)\,\tau$$

Thus

$$G_p\,(\underset{\sim}{k};\ \tau) = (i)\, e^{-i(k^2 - \frac{i}{2}\Gamma(\underset{\sim}{k};\ k^2))\tau} \qquad (3.12)$$

and

$$\tfrac{1}{2}\,\Gamma(\underset{\sim}{k};\ k^2) = \frac{2}{V^2} \sum_{\underset{\sim}{q}\underset{\sim}{q}'} \frac{\theta(P_F-q')\ \theta(|\underset{\sim}{q}'-\underset{\sim}{q}|-P_F)\ V_q^{\,2}}{\left|1 + 2\,V_{\underset{\sim}{q}}\ Q^{RPA}\ (\underset{\sim}{q};\ (\underset{\sim}{q}'-\underset{\sim}{q})^2-q'^2)\right|^2} \tag{3.13}$$

$$\times\ \pi\ \delta\left[(\underset{\sim}{k}+\underset{\sim}{q})^2 - k^2 + (\underset{\sim}{q}'-\underset{\sim}{q})^2 - q'^2\right]$$

We shall now determine the exact relationship between the rate of energy loss and $\Gamma\ (\underset{\sim}{k};\ k^2)$.

For this we go back to the general expression (2.1) for the positron propagator

$$G_p(x;\ x') = i\ \langle N|T\ \phi\ (x)\ \ \phi^{+}(x')|N\rangle \tag{3.14}$$

Now the space Fourier transform of the positron field operator is given by

$$\phi(x) = \frac{1}{\sqrt{V}} \sum_{\underset{\sim}{k}} e^{i\underset{\sim}{k}\cdot\underset{\sim}{x}}\ b_{\underset{\sim}{k}}(t) \tag{3.15}$$

where the Heisenberg time dependent operator $b_{\underset{\sim}{k}}(t)$ is related to its time independent analogue by

$$b_{\underset{\sim}{k}}(t) = e^{iHt}\ \ b_{\underset{\sim}{k}}(o)\ e^{-iHt} \tag{3.16}$$

where H is the total Hamiltonian for the combined electrons and positron system.

Taking the space Fourier transform of (3.14) we have

$$\frac{1}{V}\sum_{\underset{\sim}{k}} e^{i\underset{\sim}{k}.(\underset{\sim}{x}-\underset{\sim}{x}')} \; G_p(\underset{\sim}{k};\ \tau)$$

$$= \frac{i}{V} < N \Big| \sum_{\underset{\sim}{k}\underset{\sim}{k}'} e^{i(\underset{\sim}{k}.\underset{\sim}{x}-\underset{\sim}{k}'.\underset{\sim}{x}')} \quad x$$

$$e^{iHt}\, b_{\underset{\sim}{k}}(o)\, e^{-iHt}\, e^{iHt'}\, b_{\underset{\sim}{k}'}(o)\, e^{-iHt'} \Big| N> \qquad (3.17)$$

Now $$<N \mid e^{iHt} = e^{iE_o t} < N \mid$$

and $$e^{-iHt'}|N> = e^{-iE_o t'}|N>$$

where E_o is the ground state energy of interacting N-electron system. Thus, equation (3.17) becomes

$$\frac{1}{V}\sum_{\underset{\sim}{k}} e^{i\underset{\sim}{k}.(\underset{\sim}{x}-\underset{\sim}{x}')} \; G_p(\underset{\sim}{k};\ \tau)$$

$$= \frac{i}{V} \sum_{\underset{\sim}{k}\underset{\sim}{k}'} e^{i(\underset{\sim}{k}.\underset{\sim}{x}-\underset{\sim}{k}'.\underset{\sim}{x}')} \; e^{iE_o(t-t')}$$

$$<N|b_{\underset{\sim}{k}}(o)\, e^{-H(t-t')}\, b^{+}_{\underset{\sim}{k}'}(o)|N> \qquad (3.18)$$

Here $b^{+}_{\underset{\sim}{k}'}(o)|N>$ is the initial state of N + 1 particles with total momentum $\underset{\sim}{k}'$ and $<N|b_{\underset{\sim}{k}}(o)$ is the complex conjugate of the final state of the N + 1 particle system with momentum $\underset{\sim}{k}$. But the total momentum of the system remains the same even though a redistribution of energy and momentum may take place within the system itself.

This certainly implies that $\underset{\sim}{k} = \underset{\sim}{k}'$.

Thus

$$\frac{1}{V} \sum_{\underset{\sim}{k}} e^{i\underset{\sim}{k}.(\underset{\sim}{x}-\underset{\sim}{x}')} \; G_p(\underset{\sim}{k};\ \tau)$$

$$= \frac{i}{V} \sum_{\underset{\sim}{k}} e^{i\underset{\sim}{k}.(\underset{\sim}{x}-\underset{\sim}{x}')} \; <N|b_{\underset{\sim}{k}}(o)\, e^{-i(H-E_o)\tau}\, b^{+}_{\underset{\sim}{k}}(o)|N>$$

where $\tau = t - t' > 0$.

Hence

$$G_p(\underset{\sim}{k};\ \tau) = i\, <N|b_{\underset{\sim}{k}}(o)\, e^{-i(H-E_o)\tau}\, b^{+}_{\underset{\sim}{k}}(o)|N> \qquad (3.19)$$

Now the square of the absolute value of the time dependent positron Green's function, i.e., $|G_p(\underset{\sim}{k};\ \tau)|^2$ is the

probability that if at a time $\tau = 0$, the positron-electron system is in a state $|\underset{\sim}{k}N\rangle = b^{+}_{\underset{\sim}{k}}(o)|N\rangle$ ($|N\rangle$ being the ground state of the metal and $|\underset{\sim}{k}\rangle$ representing an incoming positron in a plane wave state of momentum $\underset{\sim}{k}$), then it will still be in this state at a later time τ.

This is easily seen from equation (3.19) since, except for a phase factor, $G_p(\underset{\sim}{k};\ \tau)$ is just the projection back on the initial state $b^{+}_{\underset{\sim}{k}}(o)|N\rangle$ of the state $e^{-iH\tau}\ b^{+}_{\underset{\sim}{k}}(o)|N\rangle$ that has developed from it in the time interval τ.

From equation (3.11) this probability is given by $e^{-\Gamma(\underset{\sim}{k};\ k^2)\tau}$.

Then the probability that the positron is not in this state at time τ, i.e., the probability that the positron will have made a transition from the state $|\underset{\sim}{k}\rangle$ to an arbitrary state $|\underset{\sim}{k}+\underset{\sim}{q}\rangle$ is

$$1 - e^{-\Gamma(\underset{\sim}{k};\ k^2)\tau}$$

Therefore, the probability per unit time that the positron will make a transition is determined by

$$\lim_{\tau \to 0} \frac{1 - e^{-\Gamma(\underset{\sim}{k};\ k^2)\tau}}{\tau} = \Gamma(\underset{\sim}{k};\ k^2) \qquad (3.20)$$

Note that as $T \to 0$ the previous condition $\Gamma\tau \ll 1$ is really no restriction at all and is automatically satisfied.

Dropping the $\underset{\sim}{q}$ summations in (3.13) gives the transition probability per unit time from the state $|\underset{\sim}{k}\rangle$ to a specific state $|\underset{\sim}{k} + \underset{\sim}{q}\rangle$.

Thus it is clear that to obtain a formula for the rate of energy loss $R[\underset{\sim}{k}]$ as a function of positron momentum $\underset{\sim}{k}$, we need to introduce inside the $\underset{\sim}{q}$ summation in (3.13) an energy transfer term $k^2 - (\underset{\sim}{k}+\underset{\sim}{q})^2$.

Hence

$$R[\underset{\sim}{k}] = \frac{4}{V^2} \sum_{\underset{\sim}{q}\underset{\sim}{q}'} \frac{\theta(P_F - q')\ \theta(|\underset{\sim}{q}'-\underset{\sim}{q}| - P_F)\ V_q^{\,2}}{|1 + 2\ V_{\underset{\sim}{q}}\ Q^{RPA}(\underset{\sim}{q};\ (\underset{\sim}{q}'-\underset{\sim}{q})^2 - q'^2)|^2}$$

$$\times \pi\ (k^2 - (\underset{\sim}{k}+\underset{\sim}{q})^2)\ \delta\left[(\underset{\sim}{k}+\underset{\sim}{q})^2 - k^2 + (\underset{\sim}{q}'-\underset{\sim}{q})^2 - q'^2\right] \tag{3.21}$$

In the next chapter, we shall be mainly concerned with the algebraic reduction of this formula for the purpose of computation.

CHAPTER 4

Algebraic Reduction and Evaluation of $R[\underset{\sim}{k}]$

The expression (3.21) for the rate of energy loss can be reduced analytically to a double integral. For the sake of convenience, we shall measure all momenta in units of the Fermi momentum P_F.

Making use of the prescription for going over from summation to integration and in the limit of infinite volume

$$\sum_{\underset{\sim}{k}} f(\underset{\sim}{k}) = \frac{V}{(2\pi)^3} \int f(\underset{\sim}{k})\, d^3k;$$

doing the transformation

$$\underset{\sim}{k} \longrightarrow \underset{\sim}{p}\, P_F$$

$$\underset{\sim}{q} \longrightarrow \underset{\sim}{q}\, P_F$$

$$\underset{\sim}{q}' \longrightarrow \underset{\sim}{q}'\, P_F$$

$$\underset{\sim}{q} \longrightarrow -\underset{\sim}{q}$$

reduces equation (3.21) to the form

$$R[\underset{\sim}{p}\ P_F] = \left(\frac{e^2}{\pi^2}\right)^2 \frac{P_F^2}{\hbar} \int_{\substack{|\underset{\sim}{q}+\underset{\sim}{q}'|>1 \\ \underset{\sim}{q}'<1}} d^3q\, d^3q' \frac{\pi\,(p^2 - (\underset{\sim}{p}-\underset{\sim}{q})^2)}{|q^2 + \alpha\, Q^{-RPA}(\underset{\sim}{q};\ (\underset{\sim}{q}'+\underset{\sim}{q})^2 - q'^2)|^2}$$

$$\times\ \delta\left[(\underset{\sim}{p}-\underset{\sim}{q})^2 - p^2 + (\underset{\sim}{q}'+\underset{\sim}{q})^2 - q'^2\right] \qquad (4.1)$$

where we have reintroduced the constants $\hbar$ and 2m set equal to 1 and e is the electronic charge. Also we have used the fact that $\delta(ax) = \frac{1}{a}\ \delta(x)$.

The parameter α is related to the usual electron density parameter r_s by $\alpha = \dfrac{r_s}{1.919\pi^2}$ and the function Q^{-RPA} to Q^{RPA} of equation (3.21) by

$$Q^{-RPA} = \left(\frac{16\pi^3}{P_F}\right)\ Q^{RPA} \qquad (4.2)$$

We shall be interested in evaluating (4.1) only for positron momenta less than or the order of 1 (i.e., Fermi momentum) since a high energy positron loses energy very rapidly as will be shown later.

For the sake of convenience in writing, we will work with $I(\underset{\sim}{p})$ rather $R[\underset{\sim}{p}\ P_F]$, where, by definition

$$I(\underset{\sim}{p}) = \left[\left(\frac{e^2}{\pi}\right)^2 \frac{P_F^2}{\hbar} \right]^{-1} R[\underset{\sim}{p}\ P_F] \qquad (4.3)$$

Therefore

$$I(\underset{\sim}{p}) = \int \frac{d^3q\ \pi\ (p^2 - (\underset{\sim}{p}-\underset{\sim}{q})^2)}{|q^2 + \alpha Q^{-RPA}(\underset{\sim}{q};\ p^2 - (\underset{\sim}{p}-\underset{\sim}{q})^2)|^2} \times$$

$$\int d^3q'\delta\left[(\underset{\sim}{p}-\underset{\sim}{q})^2 - p^2 + (\underset{\sim}{q}' + \underset{\sim}{q})^2 - q'^2\right]$$

$$|\underset{\sim}{q}+\underset{\sim}{q}'|>1$$

$$q' < 1 \qquad (4.4)$$

where we have made use of the energy conservation delta function in (4.1) which demands that $(\underset{\sim}{q}' + \underset{\sim}{q})^2 - q'^2 = p^2 - (\underset{\sim}{p}-\underset{\sim}{q})^2$ for any contribution. This makes the situation simpler since then the denominator in (4.1) can be taken out of the $\underset{\sim}{q}'$-integration and thus we obtain equation (4.4).

The integral

$$I = \int d^3q'\ \delta\left[(\underset{\sim}{p}-\underset{\sim}{q})^2 - p^2 + (\underset{\sim}{q}' + \underset{\sim}{q})^2 - q'^2\right]$$

$$|\underset{\sim}{q}+\underset{\sim}{q}'|>1 \qquad (4.5)$$

$$q'<1$$

is worked out in the Appendix A and is given by

$$I = 0 \quad \text{for } p^2 - (\underset{\sim}{p}-\underset{\sim}{q})^2 < 0$$

$$= \frac{\pi}{2q} \quad (p^2 - (\underset{\sim}{p}-\underset{\sim}{q})^2) \quad \text{for } p^2 - (\underset{\sim}{p}-\underset{\sim}{q})^2 > 0 \tag{4.6}$$

Equation (4.4) then simplifies to

$$I(\underset{\sim}{p}) = \int_{p^2-(\underset{\sim}{p}-\underset{\sim}{q})^2>0} d^3q \left(\frac{\pi^2}{2q}\right) \frac{(p^2 - (\underset{\sim}{p}-\underset{\sim}{q})^2)}{|q^2 + \alpha\, Q^{-RPA}(\underset{\sim}{q};\ p^2 - (\underset{\sim}{p}-\underset{\sim}{q})^2)|^2} \tag{4.7}$$

Now for performing the $\underset{\sim}{q}$-integration in (4.7), we fix the polar axis along the direction of $\underset{\sim}{p}$ and let the cosine of the angle between these two vectors be μ. The condition $p^2 - (\underset{\sim}{p}-\underset{\sim}{q})^2>0$, which ensures that, in any given collision with a valence electron, the positron always loses energy, can be simplified as follows.

$$p^2 - (\underset{\sim}{p}-\underset{\sim}{q})^2 > 0$$

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

$$\text{or} \quad -q + 2p\mu > 0.$$

For a fixed q,

$$\mu \geq q/2p$$

Hence $$1 \geq \mu \geq q/2p \qquad (4.8)$$

and q ranges from 0 to 2p. Incorporating these limits on the q and μ integrations, we have

$$I(\underset{\sim}{p}) = \pi^3 \int_0^{2p} q^3\, dq \int_{q/2p}^{1} d\mu \, \frac{(-q + 2p\mu)^2}{|q^2 + \alpha Q^{-\overline{RPA}}(\underset{\sim}{q};\ -q^2+2pq\mu)|^2} \qquad (4.9)$$

The demoninator in (4.9) is worked out in Appendix A, and is given by

$$\alpha^2 \pi^4 (2p\mu - q)^2 + \Big[q^2 + 2\pi\alpha \left(1 + \frac{1}{4q}\right)\left(1 - (q - p\mu)^2\right) \times$$

$$\ln \left(\frac{q + 1 - p\mu}{q - 1 - p\mu}\right)^2 + \frac{1}{4q}\left(1 - (p\mu)^2\right) \ln \left(\frac{p\mu + 1}{p\mu - 1}\right)^2\Big]^2 \qquad (4.10)$$

The first term in this expression is the square of the imaginary part and the second term is the square of the real part of the denominator in (4.9).

The integral (4.9), in its present form, cannot be reduced further analytically and was computed on the McMaster I.B.M. 7040.

The computed results bring out the following interesting features. The time required by the positron to fall to the energy level corresponding to the room temperature (.025 e.v.) is determined almost entirely by the region .1 e.v. to .025 e.v.; the time required to fall from a high energy level, say the Fermi level, to .1 e.v. is quite negligible, in comparison.

This type of behaviour of the positron can be understood by reference to Figure (7a). Here $\underset{\sim}{p}$ is the momentum of an electron in the Fermi sphere and $\underset{\sim}{q}$ is the momentum transferred to it by the positron. Then the only electrons that can be excited will be contained in the shaded region. Clearly the volume of the allowed region increases with $|\underset{\sim}{q}|$. Now a high energy positron can transfer large momentum, thereby increasing the volume of the allowed region and since the density of allowed $\underset{\sim}{k}$-vectors is constant in $\underset{\sim}{k}$-space, a larger volume implies a larger number of electrons that can be excited. Thus a high energy positron is capable of creating more electron hole-particle pairs and therefore loses energy much more rapidly than a low energy positron.

Furthermore, it is found that for low momentum transfers, the rate of energy loss of the positron in a given metal is proportional to the third power of its energy. This result is

in qualitative agreement with Lee-Whitings (1955) with the important difference, however, that the multiplying factors differ considerably. This point will be discussed in the last chapter, where we draw conclusions.

Moreover, the behaviour of the dielectric function of the electron gas as a function of momentum and energy transfer of the positron is then pertinent to our problem. The real and imaginary parts $\epsilon_1(\underset{\sim}{k},\omega)$ and $\epsilon_2(\underset{\sim}{k},\omega)$ of the dielectric function $\epsilon(\underset{\sim}{k},\omega)$ are computed as a function of $|\underset{\sim}{k}|$ and ω using the expressions (A-35) and (A-36) (worked out in Appendix A), and are plotted (for $r_s = 4$) for a number of values of $|\underset{\sim}{k}|$ (.1, .3, .5, .7, .9) (in units of k_F)) as a function of ω, in Figure 4.

Our region of importance, as indicated by the computed results, is that of low energy and low momentum transfer. We have, however, plotted ϵ_1 and ϵ_2 for large $|\underset{\sim}{k}|$ and ω, which, though not needed for the present work, may be helpful for making calculations in related fields.

In our region of interest, we find, for example, from Figure 4(a) that for $k = 0.1$ and $\omega = .02$ (=.06 e.v.), $\epsilon_1 = 260$ and $\epsilon_2 = 20$. It is also clear from expression (4.9) for $I(\underset{\sim}{p})$ that the denominator contains a term $\epsilon_1^2 + \epsilon_2^2$. The contribution

of ϵ_2^2 is, therefore, 0.6% that of ϵ_1^2. From this semi-quantitative argument, we may as well ignore ϵ_2^2 in comparison with ϵ_1^2.

In the limiting case of $\omega \to 0$, $\epsilon_2 \to 0$ and $\epsilon_1(\underset{\sim}{k},\omega)$ tends to its static limit. In fact, it was found that the same result could be obtained to better than .2% by replacing $Q^{-RPA}(\underset{\sim}{q};\ -q^2 + 2pq\mu)$ by its zero frequency limit $Q^-(\underset{\sim}{q};\ 0)$.

Thus equation (4.9) simplifies to

$$I(\underset{\sim}{p}) = \pi^3 \int_0^{2p} \frac{q^3}{6p}\, dq\, \frac{(-q+2p)^3}{|q^2 + \lambda Q^-(\underset{\sim}{q};\ 0)|^2} \qquad (4.11)$$

where $Q^-(\underset{\sim}{q};\ 0) = \left(\frac{16\pi^3}{p_F}\right) Q(\underset{\sim}{q};\ 0)$

It is proved in Appendix A that

$$Q^-(\underset{\sim}{q};\ 0) = 2\pi \left[1 - \frac{1}{2q}\left(1 - \frac{1}{4}\, q^2\right) \ln\left(\frac{q-2}{q+2}\right)^2\right] \qquad (4.12)$$

Using the well known relations

$$\alpha = r_s/1.919\pi^2$$

and $$P_F = 1.919/r_s a_o$$

where a_o is the Bohr atomic radius, the final expression for $R[\underset{\sim}{k}]$ takes the form

$$R[\underset{\sim}{k}] = \frac{A}{r_s^2} \int_0^{2p} \frac{q^3 dq\,(-q+2p)^3}{p\left[q^2 + \frac{2r_s}{1.919\pi}\left\{1 - \left(\frac{4-q^2}{8q}\right) \ln \left(\frac{q-2}{q+2}\right)^2\right\}\right]^2}$$

where $A = \left(\frac{e^2}{\pi^2}\right)^2 \cdot \frac{(1.919)^2}{\pi a_o^2} \cdot \frac{\pi^3}{6} = 3.519 \times 10^5$ erg sec.$^{-1}$ (4.13)

Here p is related to the energy E (in e.v.) of the positron by the relation

$$p = .1414 \sqrt{E}\ r_s \qquad (4.14)$$

The integral in (4.13) is computed for values of E in the range 4 e.v. to .025 e.v. and for a set of values of r_s in the complete metallic density range (2 to 5.6).

From a knowledge of the rate of energy loss of the positron, as a function of its energy, the thermalization time was calculated as follows:

Let R_i and R_{i+1} be respectively the rates of energy loss (for a fixed r_s) of the positron when it has energies E_i and E_{i+1}. Then the average rate is taken to be the arithmetic mean of the two rates, i.e., $Rav = \frac{(R_i + R_{i+1})}{2}$. Therefore the time taken by the positron to lose energy $(E_i - E_{i+1})$ is equal to

$$\tau_{i,\, i+1} = \frac{\text{Energy loss}}{\text{Average rate}} = \frac{(E_i - E_{i+1})}{Rav}$$

The energy interval was taken to be sufficiently small for a good approximation. In fact, the energy interval was taken as .005 e.v. for making calculations between the energy range 1 e.v. to .025 e.v. In general, the time taken by the positron to fall from E_1 to E_n is the sum of all partial times, i.e.,

$$\tau_T = \sum_{i=1}^{n-1} \tau_{i,\, i+1}$$

The same procedure was repeated for various values of $r_s \in (2, 5.6)$.

The thermalization time τ_T as a function of the metallic density parameter r_s and for temperature $300^{\circ}k$ is plotted in Figure 5. The graph exhibits the following important feature. The thermalization time is larger for a high density metal like aluminium than for large r_s values. This result makes sense, since higher the electron density, larger the screening, which implies weaker electron positron coupling and, therefore, a smaller rate of energy loss and hence larger thermalization time. This characteristic feature of τ_T is in contrast with the annihilation time, which is smaller for a high density metal. We shall discuss the significance of this point in the last chapter of this work.

Quantitatively $\tau_T \propto \frac{1}{r_s^2}$ (as can be read from the graph of Figure 5).

We finally make the following remark. For positron energies of the order of .1 e.v. or less, the maximum momentum transfer q entering in (4.11) is 2p. From expression (4.14) for p and for say $r_s = 2$, 2p is less than .18. (Remembering that we are expressing momenta in units of the Fermi momentum). Then,

in this case, $Q^{-}(\underset{\sim}{q};\ 0)$, to a good approximation, can be set equal to its long wavelength limit ($\underset{\sim}{q} \to 0$). This gives

$$\lim_{\underset{\sim}{q} \to 0} Q^{-}(\underset{\sim}{q};\ 0) = 4\pi$$

And, in this limiting case, the expression for $I(\underset{\sim}{p})$ reduces to a simple form.

$$I(\underset{\sim}{p}) = \frac{\pi^3 p^2}{6}\left[\frac{5}{x^2} - \frac{56}{3} + \left(4 - \frac{6}{x^2}\right) \ln\left(1 + 4x^2\right) + \frac{1}{x}\left(18 - \frac{5}{2x^2}\right) \tan^{-1} 2x\right] \qquad (4.15)$$

where $x = P/\sqrt{4\pi\alpha}$

Equation (4.15) is the Lee-Whiting's formula (1955) with the only difference that the screening parameter is, in our case, equal to $\sqrt{4\pi\alpha}\ P_F$; which is the Thomas-Fermi value for the electron gas.

CHAPTER 5

Extension to the Hubbard Approximation

We have, so far, worked in the Random Phase Approximation, which basically implies that in our calculations of the polarization part $Q(\underset{\sim}{q};\ \epsilon)$, we have limited ourselves to the inclusion of simple hole-particle bubble, shown in Figure 6. (First bubble on the right-hand side). This is surely the first and the leading term in the complete series for the polarization operator (Gell-Mann, Brueckner (1957)) and is the only important term for high densities (i.e., $r_s \ll 1$). At metallic densities ($2 < r_s < 5.6$), however, Hubbard (1957) was the first to suggest that higher order corrections may become important. His argument is based on the following physical grounds.

Let us consider an interaction process and suppose that an electron hole-particle pair is created. Now, in the R.P.A., these two quasi-particle excitations (the physical picture of a quasi electron is an electron plus its associated screening cloud) propagate freely and independently of each other, since the

screened Coulomb force acting between them is not included. This seems to be an oversimplified assumption, especially in the case of intermediate densities, where one would expect that important correlations will exist in the relative motion of the pair due to their mutual attractive interaction. This situation is analogous to that which arises in the theory of positron annihilation in metals, where it is now well established (Kahana (1963), Carbotte and Kahana (1965)) that the relative motion of the annihilating positron-electron pair is strongly correlated.

On the basis of the above arguments, Hubbard tried to include in the calculation of the polarization part $Q(\underset{\sim}{q};\ \epsilon)$ not only the R.P.A. bubble, but also the infinite set of repeated hole-particle ladders shown in Figure 6. These account for the multiple scattering of the electron hole-particle pair leading to renormalization of their relative wave function.

Hubbard did not sum this infinite set of graphs exactly, but suggested an approximate solution of the form which is related to Q^{RPA} by the equation

$$Q^{H}(\underset{\sim}{q};\ \epsilon) = \frac{Q^{RPA}(\underset{\sim}{q};\ \epsilon)}{1 - f(\underset{\sim}{q})\, Q^{RPA}(\underset{\sim}{q};\ \epsilon)} \qquad (5.1)$$

where $$f(\underset{\sim}{q}) = \frac{4\pi e^2}{q^2 + \xi\, k_F^{\,2}}$$

Here ξ is a parameter which suffered, to some extent, at least, from arbitrariness in its value.

But, recently, Crowell, Anderson and Ritche (1966) have summed the infinite set of graphs of Figure 6 numerically, using a Monte Carlo Calculation technique and conclude that, in the zero frequency limit, Hubbard's form of solution (5.1) is quite accurate, provided one chooses ξ to be of the form

$$\xi = 1.5 + 0.6\ r_s \qquad (5.2)$$

In the following formulation, we shall use this value of ξ even in the finite frequency case. This assumption is not unjustified due to the fact that, in the end, we will go over to the zero frequency limit (i.e., low energy transfer); the main point is that we are only trying to make a reasonable estimate of the effect, on the positron energy loss, of the Hubbard type corrections to the polarization part.

Using the more realistic polarization part $Q^H(\underset{\sim}{q};\ \epsilon)$, we now proceed to calculate the rate of energy loss of the positron. Replacing $Q^{RPA}(\underset{\sim}{q};\ \epsilon)$ by $Q^H(\underset{\sim}{q};\ \epsilon)$ in the expression (2.12) for the irreducible self energy operator, we have (in the region of our interest - the continuum region)

$$M^H(\underset{\sim}{k};\ \omega) = \frac{2}{V} \sum_{\underset{\sim}{q}\underset{\sim}{q}'} \theta\,(p_F - q')\,\theta\,(|\underset{\sim}{q}' - \underset{\sim}{q}| - p_F)$$

$$\times \frac{V_q^{\,2}}{(\underset{\sim}{k} - \underset{\sim}{q})^2 - \omega + (\underset{\sim}{q}' - \underset{\sim}{q})^2 - q'^2 - i\eta^+}$$

$$\times \frac{1}{\left| 1 + (2V_{\underset{\sim}{q}} - f(\underset{\sim}{q}))\, Q^{RPA}\,(\underset{\sim}{q};\ (\underset{\sim}{q}'-\underset{\sim}{q})^2 - q'^2)\right|^2}$$

(5.3)

This expression for $M^H(\underset{\sim}{k};\ \omega)$ differs from the corresponding one for $M^{RPA}(\underset{\sim}{k};\ \omega)$ (equation (2.12)) only through the appearance of function $f(\underset{\sim}{q})$ in the denominator.

Substituting from (5.1) and (5.2) in (5.3) and going through similar algebraic steps as in Chapters 3 and 4, we arrive at an expression for $I(\underset{\sim}{p})$, which instead of (4.11), now reads

$$I(\underset{\sim}{p}) = \pi^3 \int_0^{2p} \frac{q^3 dq}{6p} \quad \frac{(-q + 2p)^3}{\left[q^2 < 1 - \dfrac{.5\alpha\, \bar{Q}(\underset{\sim}{q};0)}{q^2 + \varepsilon} > + \alpha \bar{Q}(\underset{\sim}{q};\ 0)\right]^2}$$

(5.4)

The following remark is quite relevant here. It seems apparently obvious that in going from the R.P.A. to the Hubbard

scheme, one should simply replace $\tilde{Q}(\underset{\sim}{q};\ 0)$ in (4.11) by the static limit of the Hubbard polarization part. This is, however, deceptive and would lead to a different and quite incorrect result for the rate of energy loss. One must, therefore, go back to our basic equation (2.12) to reformulate a consistent theory, as we have done.

It is found from a numerical calculation that the rate of energy loss, computed with expression (5.4), yields results which are almost the same as those obtained in the R.P.A. Therefore, we will not plot our results for the thermalization time with Hubbard corrections included. This is easily understood from the fact that in the limit of $\underset{\sim}{q} \longrightarrow 0$, equation (5.4) once again reduces to the Thomas-Fermi result.

CHAPTER 6

Discussion and Conclusions

We have computed the thermalization time of positrons in metals as a function of the electron density parameter r_s in the entire range of metallic densities. The effective positron-electron interaction was treated in perturbation theory to first order but a number of approximations to the polarization part were examined. The simplest one to work with is the Random Phase Approximation. Using the dynamic dielectric function in the R.P.A., it is found that the main contribution to the thermalization time comes from the positron energy region, viz., .1 to .025 e.v.; the time taken to fall in energy say from 4 to .1 e.v. is neglegibly small, in comparison. This brought out the important fact that the region of greatest importance in determining thermalization time is the low positron energy range. Since in any given collision, the maximum energy transfer from the positron to the electron gas is its total kinetic energy and the maximum momentum

transfer is twice its momentum (this occurs for pure backward scattering), the thermalization times must depend, in an important way, only on the low energy transfer as well as low momentum transfer limit of the effective potential.

Now in the range of $\underset{\sim}{q} \rightarrow 0$, the imaginary part of the dielectric function is small and the real part attains a simple form. In fact, the real part tends towards the static limit expression. Using the static limit of the R.P.A. potential our results change by no more than .2% from those obtained by using the complete dynamic potential. In fact, both results reduce to the Fermi-Thomas limit. That is, we would obtain the same answers to better than 1% by postulating that the basic force between an electron and a positron in a metal has the form $e^2 r^{-1}$ $\exp(-\lambda_{TF} r)$ where λ_{TF} (equal to $\sqrt{4\pi\alpha}\ K_F$) is the electron gas screening length, i.e., the Fermi-Thomas parameter.

Next, the Hubbard correction to the R.P.A. was applied. This takes into account the correlations between the electron hole-particle pair created in the polarization process. These are neglected in the R.P.A. Applying such corrections, however, we find no significant change in our results. Thus, we conclude

that the formula given by Lee-Whiting is quite adequate to predict energy loss rates provided one uses the Thomas-Fermi value for the electron gas screening length.

The following word of caution is worth emphasising. It is quite true that, in the Hubbard case, $\alpha\, Q^{-H}(\underset{\sim}{q};\ 0)$ behaves like

$$\frac{4\pi\alpha(1.5 + .6\, r_s)}{1.5 + .268\, r_s}$$

in the limit $\underset{\sim}{q} \longrightarrow 0$. For example, for $r_s = 4$,

$$\alpha\, Q^{-H}\ (\underset{\sim}{q};\ 0) \cong 6\pi\alpha$$

and therefore

$$\lambda \cong \sqrt{6\pi\alpha}\quad k_F$$

which is $\sqrt{\frac{3}{2}}$ times the Fermi-Thomas value λ_{TF}. Since the thermalization time comes out $\propto \lambda^{-4}$, this will lead to value of τ_T which is 2.25 times larger than the actual value. One might argue, on this basis, that our above conclusion is undoubtedly wrong. But, as remarked in the previous chapter, one should not just replace the polarization part in the denominator of equation (4.11)

by the corrected Hubbard one, but the right value of the numerator, which contains the imaginary part of Q^H, as well as that of the denominator should be substituted in equation (2.12) and the integral reworked out.

In his calculation for sodium, Lee-Whiting used a screening parameter $\lambda = 1.02 \times 10^8$ cm^{-1}. This differs considerably from the Thomas-Fermi value of 1.477×10^8 cm^{-1} (strictly for $r_s = 4$). Thus he found a thermalization time of 3×10^{-12} sec. which is a factor of 4.5 too small. Our better calculations give $\tau_T = 1.33 \times 10^{-11}$ sec., for room temperature, which is still about 25 times smaller than the annihilation time $\tau_A = 3.4 \times 10^{-10}$ sec.

In aluminium, however, the thermalization time is comparatively longer and is equal to 5.31×10^{-11} sec., barely a factor of 4 less than $\tau_A = 2.0 \times 10^{-10}$ sec.

A significant remark is in order here. In going over from Na to Al ($r_s = 4$ to $r_s = 2$), the annihilation time τ_A <u>decreases</u> from 3.4×10^{-10} to 2.0×10^{-10} sec., whereas the thermalization time τ_T <u>increases</u> from 1.33×10^{-11} to 5.31×10^{-11} sec. Quantitatively $\tau_T \propto \frac{1}{r_s^2}$ or the thermalization rate $\propto r_s^2$.

Unfortunately, no experiments have been reported to date, which measure the thermalization time directly and therefore we cannot claim our results to have been verified experimentally.

We will, however, discuss the results of Stewart's recent effective mass experiments in the light of our present calculations. The temperatures used in his work are 110°, 300°, 400° and 600°k. Stewart's interpretation of his experimental data in sodium, particularly the point corresponding to the temperature of 110°k, is based on the general conclusion that positrons are completely thermalized even at this temperature. In fact, this is the point we have been trying to investigate so far. Our calculations show that for the highest temperature of 600°k, τ_T is 2.8×10^{-12} sec., while for the lowest temperature used, i.e., 110°k, it is $.95 \times 10^{-10}$ sec., which is only a factor of 4 less than the annihilation time. This seems to imply a small amount of non-thermalization at this temperature. This would probably not show up very significantly in Stewart's experiments and his interpretation of the positron effective temperature in terms of complete thermalization and an effective mass of about 2 stands.

As τ_T goes inversely as the square of the electron density parameter r_s, it will be interesting the investigate the state of

the positron in a high density metal and at low temperatures say at liquid Helium temperatures. We find that in aluminum for $T = 110^{o}k$, the thermalization time is 3.81×10^{-10} sec. which is about 1.9 times <u>larger</u> than $\tau_A = 2.02 \times 10^{-10}$ sec. We claim that positrons are definitely non-thermalized on annihilation even at $T = 110^{o}k$. An experiment of the type reported by Stewart and Shand may be able to detect this lack of thermalization in aluminum.

APPENDIX A

Derivation of Equation (4.10)

To derive equation (4.10), we start from the definition of the momentum frequency dependent polarization function (equation (2.8)):

$$Q(\underset{\sim}{q};\ q_o) = \frac{i}{V} \sum_{\underset{\sim}{p}} \int \frac{dp_o}{2\pi}\ G_e^o\ (\underset{\sim}{p+q};\ p_o+q_o)\ G_e^o(\underset{\sim}{p};\ p_o)$$

$$= \frac{i}{(2\pi)^4} \int G_e^o(\underset{\sim}{p+q};\ p_o + q_o)\ G_e^o(\underset{\sim}{p};\ p_o)\ d^3p\, dp_o \qquad \text{(A-1)}$$

where

$$G_e^o\ (\underset{\sim}{p};\ p_o) = \frac{1}{p_o - \epsilon_{\underset{\sim}{p}} + i\eta_p} \qquad \text{(A-2)}$$

and

$$G_e^o(\underset{\sim}{p+q};\ p_o+q_o) = \frac{1}{p_o+q_o - \epsilon_{\underset{\sim}{p+q}} + i\eta_{p+q}}$$

where η_p and η_{p+q} are quantities tending to zero such that

$$\begin{aligned} \eta_\alpha &> 0 \quad \text{for } \alpha > P_F \\ &< 0 \quad \text{for } \alpha < P_F \end{aligned} \tag{A-3}$$

Here P_F is the Fermi momentum. We first perform the p_o integration. Consider

$$\frac{1}{p_o + q_o - \epsilon_{\underset{\sim}{p+q}} + i\eta_{p+q}}$$ in the

plane of complex p_o. It has a pole at $p_o = \epsilon_{\underset{\sim}{p+q}} - q_o - i\eta_{p+q}$ which lies in the lower half plane for $|\underset{\sim}{p+q}| > p_F$ and in the upper half for $|\underset{\sim}{p+q}| < p_F$. Similarly the function $\frac{1}{p_o - \epsilon_{\underset{\sim}{p}} + i\eta_p}$ has a pole at $p_o = \epsilon_{\underset{\sim}{p}} - i\eta_p$; in the lower half for $p > p_F$ and in the upper half for $p < p_F$.

Let us consider the following four possible cases.

(a) For $|\underset{\sim}{p+q}| > p_F$ and $p > p_F$.

$$Q(\underset{\sim}{q};\ q_o) = \frac{i}{(2\pi)^4} \int \frac{d^3p\ dp_o}{(p_o + q_o - \epsilon_{\underset{\sim}{p+q}} + i\eta_{p+q})(p_o - \epsilon_{\underset{\sim}{p}} + i\eta_p)}$$

Both the poles of the integrand lie in the lower half plane. Therefore we close the contour in the upper half plane, where the function is analytic. Thus there is no contribution to $Q(\underset{\sim}{q};\ q_o)$ in this domain.

(b) Similarly for $|\underset{\sim}{p}+\underset{\sim}{q}| < p_F$ and $p < p_F$, we again get zero.

(c) For $|\underset{\sim}{p}+\underset{\sim}{q}| > p_F$ and $p < p_F$.

In this region, the contribution to

$$Q(\underset{\sim}{q};\ q_o) \text{ is } \frac{i}{(2\pi)^4} \int \frac{d^3p\, dp_o}{(p_o+q_o - \epsilon_{\underset{\sim}{p}+\underset{\sim}{q}} + io^+)\,(p_o - \epsilon_{\underset{\sim}{p}} - io^+)}$$

We close the contour in the upper half plane, where

$$\frac{1}{p_o - \epsilon_{\underset{\sim}{p}} - io^+}$$

has a pole $p_o = \epsilon_{\underset{\sim}{p}} + io^+$. Then using the residue theorem, we have

$$Q(\underset{\sim}{q};\ q_o) = \frac{(2\pi i)(i)}{(2\pi)^4} \int \frac{d^3p}{\epsilon_{\underset{\sim}{p}} + q_o - \epsilon_{\underset{\sim}{p+q}} + io^+}$$

$$= \frac{-1}{(2\pi)^3} \int \frac{d^3p}{\epsilon_{\underset{\sim}{p}} + q_o - \epsilon_{\underset{\sim}{p+q}} + io^+} \qquad \text{(A-4)}$$

(d) Further for $|\underset{\sim}{p} + \underset{\sim}{q}| < p_F$, $p > p_F$, we obtain in a similar way a contribution of

$$\frac{-1}{(2\pi)^3} \int \frac{d^3p}{\epsilon_{\underset{\sim}{p+q}} - \epsilon_{\underset{\sim}{p}} - q_o + io^+} \qquad \text{(A-5)}$$

In order to write equations (A-4) and (A-5) in a compact form, let us introduce the step functions:

$$f_{\underset{\sim}{p}} = 1 \qquad \text{for } p < p_F$$

$$= 0 \qquad \text{for } p > p_F$$

and (A-6)

$$f_{p+q} = 1 \qquad \text{for } |\underset{\sim}{p+q}| < p_F$$

$$= 0 \qquad \text{for } |\underset{\sim}{p+q}| > p_F$$

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Then equations (A-4) and (A-5) can be written in a combined form as

$$Q(\underset{\sim}{q};\ q_o) = \frac{1}{(2\pi)^3}\left[\int\left\{\frac{f_{\underset{\sim}{p}}(1 - f_{\underset{\sim}{p}+\underset{\sim}{q}})}{\epsilon_{\underset{\sim}{p}+\underset{\sim}{q}} - \epsilon_{\underset{\sim}{p}} - q_o - io^+} - \right.\right. \tag{A-7}$$

$$\left.\left.\frac{f_{\underset{\sim}{p}+\underset{\sim}{q}}(1 - f_{\underset{\sim}{p}})}{\epsilon_{\underset{\sim}{p}+\underset{\sim}{q}} - \epsilon_{\underset{\sim}{p}} - q_o + io^+}\right\} d^3p\right]$$

For further simplification, we make the following transformations in the second integral of (A-7).

Let $\underset{\sim}{p} + \underset{\sim}{q} \longrightarrow \underset{\sim}{p}$

$$\underset{\sim}{p} \longrightarrow \underset{\sim}{p} - \underset{\sim}{q}$$

and then set $\underset{\sim}{p} \longrightarrow -\underset{\sim}{p}$ to get

$$Q(\underset{\sim}{q};\ q_o) = \frac{1}{(2\pi)^3}\left[\int\left\{\frac{1}{\epsilon_{\underset{\sim}{p}+\underset{\sim}{q}} - \epsilon_{\underset{\sim}{p}} - q_o - io^+} + \frac{1}{\epsilon_{\underset{\sim}{p}+\underset{\sim}{q}} - \epsilon_{\underset{\sim}{p}} + q_o + io^+}\right\}\right.$$

$$\left. \times f_{\underset{\sim}{p}}(1 - f_{\underset{\sim}{p}+\underset{\sim}{q}})\, d^3p\right] \tag{A-8}$$

In order to determine the real and imaginary parts of $Q(\underset{\sim}{q};\ q_o)$, we make use of the relation

$$\lim \frac{1}{x \pm io^+} = PP(\frac{1}{x}) \mp i\pi\delta(x) \qquad \text{(A-9)}$$

Then

$$\mathrm{Re}Q(\underset{\sim}{q};\ q_o) = \frac{1}{(2\pi)^3}\left[\int PP\left\{\frac{1}{\epsilon_{\underset{\sim}{p}+\underset{\sim}{q}} - \epsilon_{\underset{\sim}{p}} - q_o} + \frac{1}{\epsilon_{\underset{\sim}{p}+\underset{\sim}{q}} - \epsilon_{\underset{\sim}{p}} + q_o}\right\}\right.$$

$$\left. d^3p\ f_p\ (1 - f_{p+q})\right] \qquad \text{(A-10)}$$

and

$$\mathrm{Im}\ Q(\underset{\sim}{q};\ q_o) = \frac{\pi}{(2\pi)^3}\int d^3p\ f_p(1-f_{p+q})\left[\delta(\epsilon_{\underset{\sim}{p}+\underset{\sim}{q}} - \epsilon_{\underset{\sim}{p}} - q_o)\right.$$

$$\left. + \delta\ (\epsilon_{\underset{\sim}{p}+\underset{\sim}{q}} - \epsilon_{\underset{\sim}{p}} + q_o)\ \right] \qquad \text{(A-11)}$$

Having separated out the real and imaginary parts of the dynamic polarization function, we now proceed to obtain explicit expressions for them. Owing to the conditions imposed on the $\underset{\sim}{p}$-integration and further additional δ-function restrictions imposed

on the imaginary part, we have to determine their values separately in different regions of $\underset{\sim}{q}$.

The three possible regions are

$$|\underset{\sim}{q}| \in (0, p_F), \quad |\underset{\sim}{q}| \in (p_F, 2p_F), \quad |\underset{\sim}{q}| > 2p_F.$$

To start with we study the real part of $Q(\underset{\sim}{q};\ q_o)$

Case (a) $\quad |\underset{\sim}{q}| \in (0, p_F)$

From equation (A-10), we find that for any contribution, we must have

$$|\underset{\sim}{p}+\underset{\sim}{q}| > p_F, \quad p < p_F.$$

These coditions limit the region of $\underset{\sim}{p}$-integration to the shaded one shown in Figure 7a.

In Figure 7a, we have drawn two circles each of radius p_F with their centres separated by a distance q. As $q < p_F$, the circles must overlap. Because of spherical symmetry we work in spherical coordinates.

Let the polar axis be taken along the $\underset{\sim}{q}$ direction. The region of interest in the shaded region between the parallel planes B and C. Here B is the right bisector plane of q and C is the plane at a distance $q + p_F$ from O.

The ϕ-integration gives 2π. The range of p is $(p_F - q, p_F)$.

The limits on the θ-integration are determined as follows. Fix any arbitrary value of p in the allowed range. With O' as centre and with this arbitrarily chosen p as radius draw an arc of a circle, which cuts the O-circle at D. Thus $OD = |\underset{\sim}{p}+\underset{\sim}{q}| = p_F$ and $O'D = P$. Then from the Δ OO'D

$$(\underset{\sim}{p}+\underset{\sim}{q})^2 = (p_F)^2 = (\underset{\sim}{q})^2 + 2\underset{\sim}{q}.\underset{\sim}{p} + (p)^2$$

$$= q^2 + p^2 + 2pq\mu$$

Therefore, for a fixed p, minimum value of μ is

$$\frac{p_F^2 - q^2 - p^2}{2pq}$$

The upper limit of μ is 1, which is the case when $\underset{\sim}{p}$ and $\underset{\sim}{q}$ are in the same direction.

Hence

$$\mu \in \left(\frac{p_F^2 - q^2 - p^2}{2pq}, \; 1\right).$$

Then

$$\mathrm{Re}Q(\underset{\sim}{q};\; q_o) = \frac{2\pi}{(2\pi)^3} \int_{p_F-q}^{p_F} p^2 dp \int_{\frac{p_F^2-q^2-p^2}{2pq}}^{1} d\mu \left(\frac{1}{q^2+2pq\mu - q_o} + \frac{1}{q^2+2pq\mu+q_o}\right) \tag{A-12}$$

Performing the μ-integration we obtain

$$\begin{aligned}
\mathrm{Re}Q(\underset{\sim}{q};\; q_o) = \frac{2\pi}{(2\pi)^3} \int_{p_F-q}^{p_F} p^2 \Big\{ & \frac{1}{2pq} \ln (q^2 + 2pq - q_o) \\
& + \ln (q^2 + 2pq + q_o) \\
& - \ln (p_F^2 - p^2 - q_o) \\
& - \ln (p_F^2 - p^2 + q_o) \Big\} \; dp
\end{aligned}$$

$$= \frac{\pi}{q} \int_{p_F-q}^{p_F} pdp \Big\{ \ln (q^2 + 2pq - q_o) + \ln (q^2 + 2pq + q_o) - \ln (p_F^2 - p^2 - q_o) - \ln (p_F^2 - p^2 + q_o) \Big\} \tag{A-13}$$

Making use of the formulae

$$\int x \ln (a + bx)\, dx = \frac{b^2 x^2 - a^2}{2b^2} \ln (a + bx) + \frac{ax}{ab} - \frac{x^2}{4}$$

and

$$\int x \ln |(a^2-x^2)|dx = \frac{1}{2}\left[(x^2-a^2) \ln |a^2-x^2| - x^2\right] \qquad \text{(A-14)}$$

one obtains on performing the p-integration,

$$\mathrm{Re}Q(\underset{\sim}{q};\ q_o) = \frac{\pi}{2q} \frac{1}{(2\pi)^3}\left[2qp_F + (p_F^2 - \frac{(q^2-q_o)^2}{4q^2})\ln \left| \frac{2qp_F+q^2-q_o}{2qp_F-q^2+q_o}\right|\right.$$

$$\left. + (p_F^2 - \frac{(q^2+q_o)^2}{4q^2}) \ln \left|\frac{2qp_F + q^2 + q_o}{2qp_F - q^2 - q_o}\right|\right]$$

$$= \frac{\pi p_F}{(2\pi)^3}\left[1 + \frac{p_F}{2q} (1 - x^2) \ln \left|\frac{1+x}{1-x}\right| - \frac{p_F}{2q} (1-y^2)\ln\left|\frac{1+y}{1-y}\right| \right]$$

(A-15)

where

$$x = \frac{q_o}{2qp_F} + \frac{q}{2p_F}$$

$$y = \frac{q_o}{2qp_F} - \frac{q}{2p_F} \quad . \qquad \text{(A-16)}$$

Case (b) $|\underset{\sim}{q}| \in (p_F, 2p_F)$.

We proceed in the same way as before. The total domain of integration can now be split up into two domains, viz., a circle of radius $q - p_F$ and the remaining shaded region between the planes B and C. Clearly, from the Figure 7b, μ varies for the second region between

$$\left(\frac{p_F^2 - p^2 - q^2}{2pq}, \quad 1\right)$$

and $$p \in (q - p_F, p_F).$$

Thus, we obtain

$$\mathrm{Re}Q(\underset{\sim}{q};\ q_o) = \frac{1}{(2\pi)^3}\ 2\pi\ \Bigg[\int_0^{q-p_F} p^2\,dp \int d\mu \left(\frac{1}{q^2+2pq\mu - q_o} + \frac{1}{q^2 + 2pq\mu + q_o}\right)$$

$$+ \int_{q-p_F}^{p_F} p^2 dp \int_{\frac{p_F^2-p^2-q^2}{2pq}}^{+1} d\mu \left(\frac{1}{q^2+2pq\mu-q_o} + \frac{1}{q^2 + 2pq\mu + q_o}\right) \Bigg] \qquad \text{(A-17)}$$

The integrations are trivial and one finds, on simplification,

$$\mathrm{Re}Q(\underset{\sim}{q};\ q_o) = \frac{\pi p_F}{(2\pi)^3}\left[1 + \frac{p_F}{2q}\ (1-x^2)\ \ln\left|\frac{1+x}{1-x}\right| - \frac{p_F}{2q}\ (1-y^2)\ \ln\left|\frac{1+y}{1-y}\right|\right] \tag{A-18}$$

which is the same as equation (A-15).

Case (c) $|\underset{\sim}{q}| > 2\ p_F$

This is the simplest of the three cases. The ϕ-integration gives 2π. p and μ range over the complete circle (Figure 7c).

We have thus

$$\mathrm{Re}Q(\underset{\sim}{q};\ q_o) = \frac{1}{(2\pi)^3}\ 2\pi \int_0^{p_F} p^2 dp \int_{-1}^{+1} d\mu \left\{\frac{1}{q^2+2pq\mu - q_o} + \frac{1}{q^2+2pq\mu+q_o}\right\} \tag{A-19}$$

The integrations are performed without much labour. One finally obtains the same expression for $\mathrm{Re}Q(\underset{\sim}{q};\ q_o)$ as in (A-15) or (A-18).

Thus, we have the general expression for the real part of the polarization function in the Random Phase Approximation

$$\mathrm{Re}Q(\underset{\sim}{q};\ q_o) = \frac{\pi p_F}{(2\pi)^3}\left[1 + \frac{p_F}{2q}\ (1-x^2)\ \ln\left|\frac{1+x}{1-x}\right| - \frac{p_F}{2q}\ (1-y^2)\ \times \right.$$

$$\left. \ln\left|\frac{1+y}{1-y}\right| \right] \qquad \text{(A-20)}$$

In the second part of this appendix we work out the imaginary part of $Q(\underset{\sim}{q};\ q_o)$ in the R.P.A.

As already remarked, the conditions for integration for Im $Q\ (\underset{\sim}{q};\ q_o)$ are similar to those for $\mathrm{Re}Q(\underset{\sim}{q};\ q_o)$ with the difference, however, that the δ-function further limits the domain of integration.

For the sake of convenience, we consider the case of positive frequencies only and later on generalize the results to both the positive and negative frequencies. With this in mind, we write equation (A-11) for $q_o > 0$,

$$\text{Im } Q\ (\underset{\sim}{q};\ q_o) = \frac{\pi}{(2\pi)^3}\ I_1 \qquad \text{(A-21)}$$

where

$$I_1 = \int f_p \, (1 - f_{p+q}) \, \delta \, [\epsilon_{\underset{\sim}{p+q}} - \epsilon_{\underset{\sim}{p}} - q_o] \, d^3p \qquad \text{(A-22)}$$

$$= \int_{\substack{|\underset{\sim}{p+q}|>p_F \\ p<p_F}} \delta \, (q^2 + 2pq\,\mu - q_o) \, d^3p \qquad \text{(A-23)}$$

where μ is the cosine of the angle between $\underset{\sim}{p}$ and $\underset{\sim}{q}$.

For δ-function to click, we should have

$$p\,\mu = \frac{q_o - q^2}{2q} \qquad \text{(A-24)}$$

We evaluate I_1 in the three regions, as before.

Case (a) $|\underset{\sim}{q}| < p_F$.

Consider Figure 7d.

Take a point D on the curved line of the left circle, which is enclosed between the planes B and C. From the $\Delta OO'D$

$$p_F^2 = p^2 + q^2 + 2pq\,\mu$$

or
$$\mu = \frac{p_F^2 - q^2 - p^2}{2pq}$$

Hence the range of μ is

$$\left(\frac{p_F^2 - q^2 - p^2}{2pq}, \; +1\right)$$

But, due to the δ-function restrictions, the ranges of p will be different in the two shaded regions, i.e., between planes A and C and that between planes A and B.

Now between the planes A and C, the δ-function demands that

$$p_F - q \leq \frac{q_o - q^2}{2q} \leq p_F$$

or

$$2qp_F - q^2 \leq q_o \leq q^2 + 2q\,p_F$$

or

$$q_o \in (2qp_F - q^2,\; q^2 + 2qp_F)$$

and in this range of q_o, $p \in \left(\frac{q_o - q^2}{2q}, \; p_F\right)$.

Hence

$$I_1 = \int_{\frac{q_o - q^2}{2q}}^{p_F} p^2 dp \int_{\frac{p_F^2 - q^2 - p^2}{2pq}}^{1} \delta(q^2 + 2pq\mu - q_o)\; d\mu$$

$$= \frac{\pi}{2q}\left[p_F^2 - \left(\frac{q_o - q^2}{2q}\right)^2\right] \quad \text{for } q_o \in (2qp_F - q^2,\ 2qp_F + q^2)$$

(A-25)

Now consider the region between the planes A and B. Imposing δ-function restrictions, one finds that

$$-q/2 \leqslant \frac{q_o - q^2}{2q} \leqslant p_F - q$$

or

$$0 \leqslant q_o \leqslant 2qp_F - q^2$$

and in this range of $q_o \in (0,\ 2qp_F - q^2)$, μ again ranges between $\left(\frac{p_F^2 - q^2 - p^2}{2pq},\ +1\right)$ but the p-integration range is a little bit complicated and is obtained as follows:

Draw DE $\perp^r$ on the q-axis.

Then, we have

$$p_F^2 = (q + p\mu)^2 + a^2$$

and

$$p^2 = (p\mu)^2 + a^2$$

Therefore

$$p_F^2 - p^2 = (q + p\mu)^2 - p^2$$

$$= q^2 + 2pq\mu$$

$$= q^2 + 2pq\left(\frac{q_o - q^2}{2pq}\right)$$

$$= q_o$$

or

$$p = \sqrt{p_F^2 - q_o} \qquad \text{(A-26)}$$

Hence for $q_o \in (0, 2qp_F - q^2)$

$$I_1 = 2\pi \int_{(p_F^2 - q_o)^{1/2}}^{p_F} p^2 dp \int_{\frac{p_F^2 - q^2 - p^2}{2pq}}^{+1} d\mu\, \delta(q^2 + 2pq\mu - q_o)$$

$$= \frac{\pi q_o}{2q} \qquad \text{(A-27)}$$

and in the region $q_o > q^2 + 2q\, p_F$

$$I_1 = 0 \qquad \text{(A-28)}$$

Case (b) $|\underset{\sim}{q}| \in (p_F, 2p_F)$.

In this case the two spheres again overlap. The contribution to the integral comes only from the shaded region, shown in Figure 7e.

The situation is similar to that in the previous case of $|\underset{\sim}{q}| < p_F$. The results are the same as (A-25), (A-27) and (A-28) for the three regions of q_o, discussed above.

Case (c) $|\underset{\sim}{q}| > 2p_F$

The spheres do not overlap in this case. Except for the δ-function, the whole of the sphere should be the integration range.

However, for the δ-function to click we must have

$$- p_F \leq \frac{q_o - q^2}{2q} \leq p_F$$

or

$$q^2 - 2qp_F \leq q_o \leq q^2 + 2qp_F.$$

Once again, for $q_o > q^2 + 2qp_F$, there is no contribution. In contrast to the two cases discussed above, I_1 vanishes for $q_o < q^2 - 2qp_F$.

Thus the only region of q_o that contributes is

$$q_o \in (q^2 - 2qp_F, \quad q^2 + 2qp_F).$$

In this region

$$I_1 = 2\pi \int_{\frac{q_o - q^2}{2q}}^{p_F} p^2 dp \int_{-1}^{+1} d\mu \, \delta(q^2 + 2qp\mu - q_o)$$

$$= 2\pi \int_{\frac{q_o - q^2}{2q}}^{p_F} p^2 dp \quad \frac{1}{2qp}$$

$$= \frac{\pi}{2q} \left[p_F^2 - \left(\frac{q_o - q^2}{2q} \right)^2 \right] \qquad \text{(A-29)}$$

Summing up, we write down the general results for the real and imaginary parts of the polarization function ($q_o > 0$)

$$\mathrm{Re}Q(\underset{\sim}{q};\ q_o) = \frac{\pi p_F}{(2\pi)^3}\left\{1 + \frac{p_F}{4q}(1 - x^2)\ln\left(\frac{1+x}{1-x}\right)^2 - \frac{p_F}{4q}(1 - y^2)\ln\left(\frac{1+y}{1-y}\right)^2\right\} \qquad \text{(A-30)}$$

and

$$\mathrm{Im}Q(\underset{\sim}{q};\ q_o) = \frac{\pi}{(2\pi)^3}\cdot\frac{\pi q_o}{2q} \qquad \text{for } q < 2p_F \text{ and } q_o \leq |2qp_F - q^2|$$

$$= \frac{\pi}{(2\pi)^3}\cdot p_F^2\cdot\frac{\pi}{2q}\times(1-y^2) \qquad \text{for } |2qp_F - q^2| \leq q_o \leq 2qp_F + q^2$$

$$= 0 \qquad \text{for } q > 2p_F \text{ and } q_o < |q^2 - 2qp_F|$$

$$= 0 \qquad \text{for } q_o > q^2 + 2qp_F \qquad \text{(A-31)}$$

where x and y are given by (A-16).

It can be easily seen from equation (A-11) that one obtains the same results for $\mathrm{Im}Q(\underset{\sim}{q};\ q_o)$ for negative as for positive q_o.

Now we express all momenta in units of Fermi momentum p_F. This implies that we make the transformation

$$\underset{\sim}{q} \longrightarrow \underset{\sim}{q}\ p_F,$$

$$q_o \longrightarrow q_o\ p_F^2.$$

Making these transformations in equations (A-30) and (A.31) and putting $q_o = -q^2 + 2pq\,\mu$ (on comparison with value of q_o in equation (4.9)) in the transformed equations (A-30) and (A-31), we obtain in the region of low energy transfers ($q_o \leq |\, q^2 - 2q\,|$ - our region of interest).

$$\left|q^2 + \alpha Q^{-RPA}\ (\underset{\sim}{q};\ -q^2+2pq\mu)\ \right|^2 = (q^2 + \alpha\,\mathrm{Re}\ Q^{-RPA})^2 + (\alpha\,\mathrm{Im}\ Q^{-RPA})^2$$

$$= \Big[q^2 + 2\pi\alpha\Big\{1 + \frac{1}{4q}(1-(q-p\mu)^2)\ln\Big(\frac{q+1-p\mu}{q-1-p\mu}\Big)^2 + \frac{1}{4q}(1-(p\mu)^2)\ln\Big(\frac{\mu p+1}{\mu p-1}\Big)^2\Big\}\Big]^2 + \alpha^2\pi^4(2p\mu-q)^2$$

(A-32)

which is the desired equation (4.10). When $-q^2 + 2pq/\mu = 0$ we get $Q^-(\underset{\sim}{q};\ 0) = 2\pi \left[1 - \frac{1}{2q}\left(1 - \frac{1}{4}q^2\right) \ln \left(\frac{q-2}{q+2}\right)^2\right]$ which is equation (4.12).

It is now a matter of two steps to prove equation (4.6). Setting $q_o = p^2 - (\underset{\sim}{p}-\underset{\sim}{q})^2$ in equation (4.6), we have

$$I = \int_{\substack{|\underset{\sim}{q}'+\underset{\sim}{q}|>1 \\ q'<1}} d^3q'\ \delta\left[(\underset{\sim}{q}' + \underset{\sim}{q})^2 - q'^2 - q_o\right] \qquad (A\text{-}33)$$

It may be remarked that all momenta have been expressed in units of Fermi momentum p_F.

Now, obviously, $(\underset{\sim}{q}' + \underset{\sim}{q})^2 - q'^2 > 0$. Therefore, for the argument of the δ-function to vanish, we should have $q_o > 0$.

Hence

$$I = 0 \qquad \text{for } p^2 - (\underset{\sim}{p}-\underset{\sim}{q})^2 < 0$$

Now, in our region of interest, ($q < 1$), q_o is small. In fact, the range of q_o can be taken to be $(0, 2q-q^2)$. Using equation (A-27), one finds

$$I = \frac{\pi}{2q} \cdot q_o$$

$$= \frac{\pi}{2q} \left(p^2 - (\underset{\sim}{p}-\underset{\sim}{q})^2\right) \text{ for } q_o > 0. \qquad \text{(A-34)}$$

which is the required equation (4.6).

Expressions for $\epsilon_1(\underset{\sim}{k};\ \omega)$ and $\epsilon_2(\underset{\sim}{k};\ \omega)$

The real and imaginary parts of the dielectric function are given by equation (2.9):

$$\epsilon_1(q;\ q_o) = 1 + 2\, V_{\underset{\sim}{q}}\, \mathrm{Re}\, Q^{RPA}(\underset{\sim}{q};\ q_o)$$

$$\epsilon_2(q;\ q_o) = 2\, V_{\underset{\sim}{q}}\, I_m\, Q^{RPA}(\underset{\sim}{q};\ q_o)$$

With the help of equations (A-30) and (A-31) and expressing all momenta in units of Fermi momentum, i.e, making

the transformations $\underset{\sim}{q} \to \underset{\sim}{k}\, k_F$ and $q_o \to \omega\, k_F^2$, we obtain

$$\epsilon_1(\underset{\sim}{k};\ \omega) = 1 + \frac{2r_s}{\pi(1.919)k^2}\left[1 + \frac{1}{4k}\left(1 - \left(\frac{\omega}{2k} + \frac{k}{2}\right)^2\right) \times \ln\left\{\frac{1 + \left(\frac{\omega}{2k} + \frac{k}{2}\right)}{1 - \left(\frac{\omega}{2k} + \frac{k}{2}\right)}\right\}^2 - \frac{1}{4k}\left(1 - \left(\frac{\omega}{2k} - \frac{k}{2}\right)^2\right) \times \ln\left\{\frac{1 + \left(\frac{\omega}{2k} - \frac{k}{2}\right)}{1 - \left(\frac{\omega}{2k} - \frac{k}{2}\right)}\right\}^2\right] \qquad \text{(A-35)}$$

and

$$\epsilon_2(\underset{\sim}{k};\ \omega) = 0 \quad \text{for} \quad \omega > k^2 + 2k$$

$$= 0 \quad \text{for} \quad k > 2 \quad \text{and} \quad \omega < |k^2 - 2k|$$

$$= \frac{\omega r_s}{1.919\, k^3} \quad \text{for } k < 2 \text{ and } \omega < |k^2 - 2k| \qquad \text{(A-36)}$$

$$= \frac{r_s}{1.919\, k^3}\left\{1 - \left(\frac{\omega}{2k} - \frac{k}{2}\right)^2\right\}$$

$$\text{for } |k^2 - 2k| < \omega < 2k + k^2$$

where we have made use of the equations $v_{\underset{\sim}{q}} = \frac{4\pi e^2}{q^2}$ and

$k_F r_s = 1.919$ (r_s is expressed in atomic units), and remembering that $e^2 = 2$, $\hbar = 2m = 1$ in atomic units.

APPENDIX B

Expression for Γ (p - 18)

On taking out the energy transfer term from expression (4.1) for the rate of energy loss, one obtains an expression for $\Gamma(\underset{\sim}{p})$. Hence, the width of the peaked function (i.e., integrand without the exponential in (3.8)) in units of energy is given by

$$\Gamma(\underset{\sim}{p}) = \left(\frac{e^2}{\pi^2}\right)^2 \frac{p_F^2}{\hbar} \times \frac{2m}{p_F^2 \hbar^2} \times \pi \times \hbar$$

$$\times \int_{\substack{|\underset{\sim}{q}+\underset{\sim}{q}'|>1 \\ q'<1}} \frac{d^3q \; d^3q'}{|q^2 + \mathcal{L}\, Q^{\text{-RPA}}(\underset{\sim}{q};\ (\underset{\sim}{q}'+\underset{\sim}{q})^2 - q^2)|^2}$$

$$\times \delta\left[(\underset{\sim}{p}-\underset{\sim}{q})^2 - p^2 + (\underset{\sim}{q}' + \underset{\sim}{q})^2 - q'^2\right] \qquad \text{(B-1)}$$

$$= \frac{e^4}{\pi^3} \cdot \frac{2m}{\hbar^2} \cdot \int_{p^2-(\underset{\sim}{p}-\underset{\sim}{q})^2>0} \frac{d^3q \left(\frac{\pi}{2q}\right) \left(p^2 - (\underset{\sim}{p}-\underset{\sim}{q})^2\right)}{\left|q^2 + \lambda Q^{-RPA}\left(\underset{\sim}{q};\ p^2-(\underset{\sim}{p}-\underset{\sim}{q})^2\right)\right|^2} \qquad \text{(B-2)}$$

where we have made use of (A-34).

In (B-2), the ϕ integration gives 2π. Further, the condition $p^2 - (\underset{\sim}{p}-\underset{\sim}{q})^2>0$ implies that $\mu \in (q/2p, 1)$. q ranges from 0 to 2p.

Then, in the static limit,

$$\Gamma(\underset{\sim}{p}) = \frac{e^4}{\pi^3} \cdot \frac{2m}{\hbar^2} \cdot \pi^2 \int_0^{2p} \frac{q^2\, dq}{\left(q^2 + \lambda Q^{-}(\underset{\sim}{q};\ o)\right)^2}$$

$$\times \int_{q/2p}^{+1} (-q + 2p\mu)\, d\mu \ .$$

$$\text{or } \Gamma(\underset{\sim}{p}) = A' \int_0^{2p} \frac{q^2 \left(-q + p + \frac{q^2}{4p}\right) dq}{\left(q^2 + \frac{2 r_s}{1.919\pi}\left(1 - \left(\frac{4-q^2}{8q}\right) \ln\left(\frac{q-2}{q+2}\right)^2\right)^2\right)} \qquad \text{(B-3)}$$

(in e.v.)

where $A' = \frac{e^4}{\pi} \cdot \frac{2m}{\hbar^2} \cdot \frac{1}{1.6 \times 10^{-12}}$ e.v.

$$= 17.34 \text{ e.v.} \qquad \text{(B-4)}$$

Here $p = .1414 \sqrt{E}\ r_s$ (E in e.v.).

The expression (B-3) was employed for computation of Γ as a function of r_s and E.

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CAPTION TO FIGURES

Figure 1 Positron self-energy operator in the Random Phase Approximation (R.P.A.). Note that the first graph in (1a) is really zero since it involves $G_p^o(x;\ x')$ for the time ordering $t' - t > 0$ $(\longrightarrow 0)$. It is included, nevertheless, because it is the natural first member of the infinite series shown. In (1b) the wiggly dynamic interaction line stands for the effective potential in R.P.A.

Figure 2 The integral equation for the effective potential $\mu(x;\ x')$ in the R.P.A.

Figure 3 (a) Singularities of $M\ (\underset{\sim}{k};\ \omega)$

(b) Contour used for integrating equation (3.1)

(c) Graph of the integrand in equation (3.10)

Figure 4 (a), (b), (c), (d), and (e):

Graphs for the real and imaginary parts (ϵ_1 and ϵ_2 respectively) of the dielectric function $\epsilon(\underset{\sim}{k};\ \omega)$ in R.P.A. for $r_s = 4$ for values of $k = .1, .3, .5, .7, .9$ (in units of Fermi momentum) respectively.

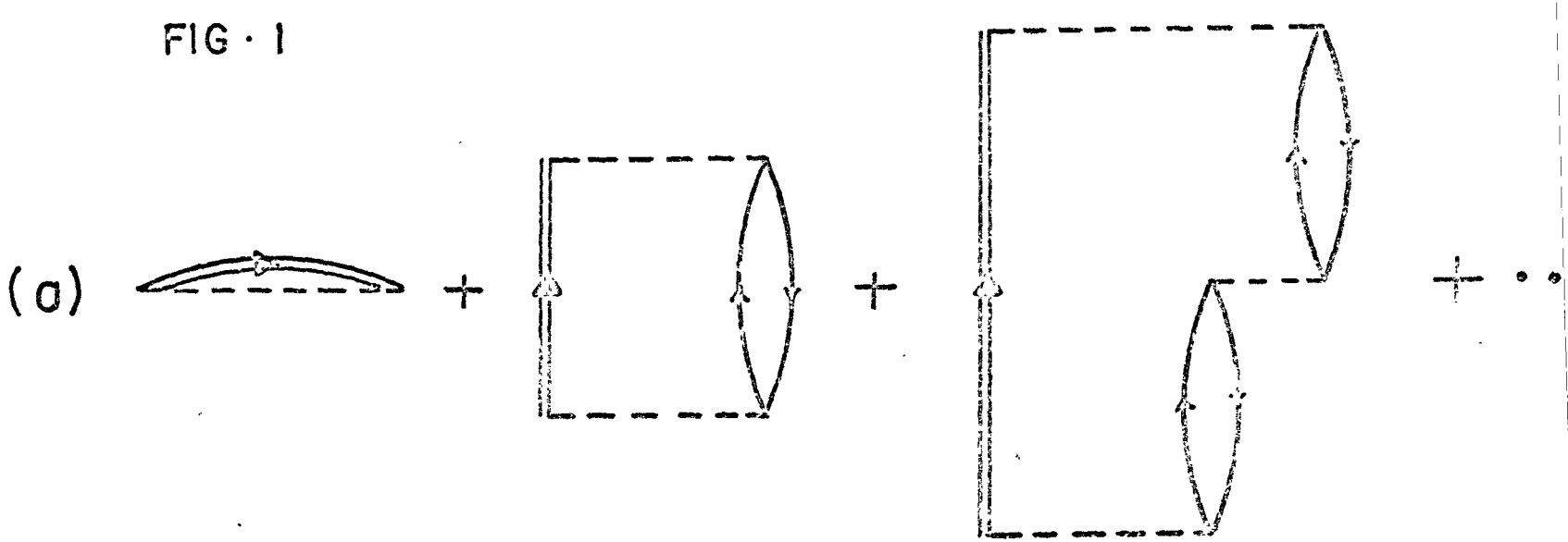
Figure 5 The thermalization time τ_T as a function of the electron gas density parameter r_s for temperature T = 300°k.

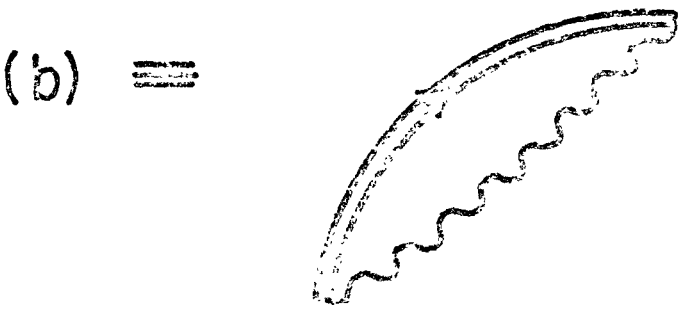
Figure 6 Graphs which are included in the calculation of the polarization function $Q(\underset{\sim}{k};\ \epsilon)$ in the Hubbard approximation.

Figure 7 Regions of integration of expressions (A-10) and (A-11) for real and imaginary parts of the polarization function. (a), (b), (c) correspond to the case of $|\underset{\sim}{q}| < (0, p_F)$, $\epsilon(p_F, 2p_F)$, $|\underset{\sim}{q}| > 2p_F$ in the case of Re $Q(\underset{\sim}{q};\ q_o)$ and (d), (e), (f) correspond to the same ranges of $|\underset{\sim}{q}|$ for Im $Q(\underset{\sim}{q};\ q_o)$.

Table 1 The peak width Γ (e.v.) of the integrand of Equation (3.8) as a function of the positron energy (.1e.v. - .01 e.v.) for values of r_s (2-6 in a.u.).

FIG · 1





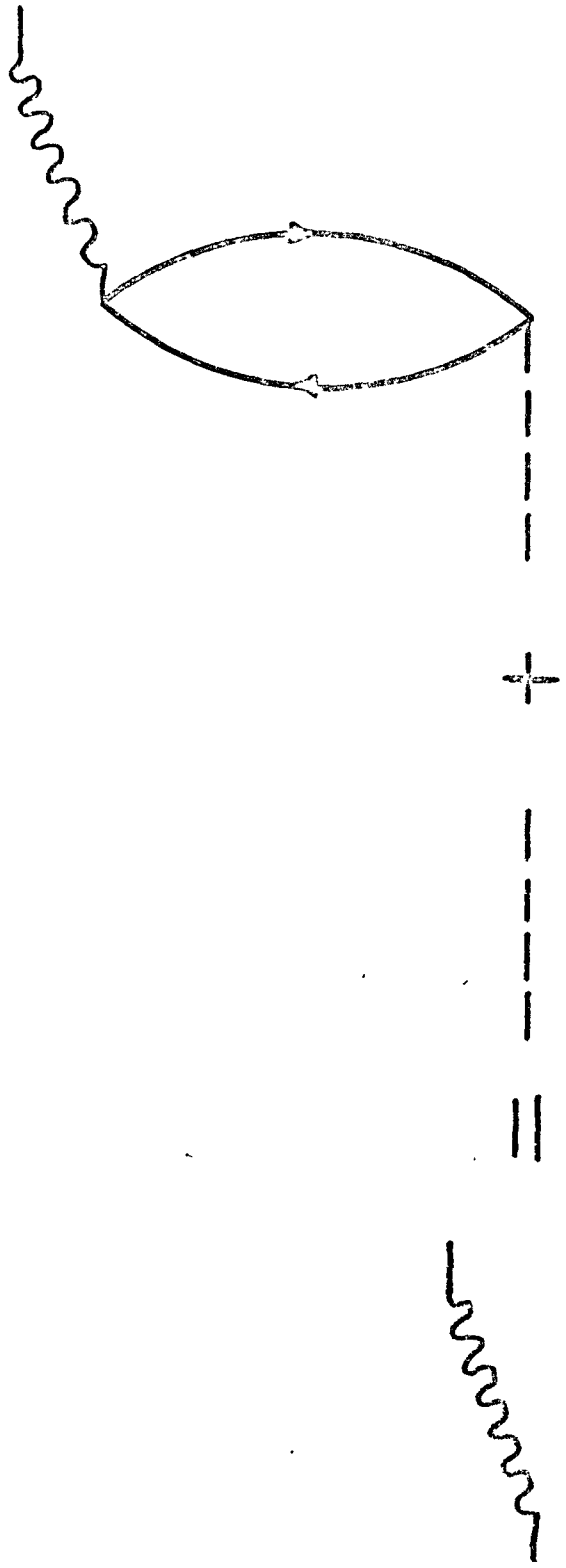


Fig.2

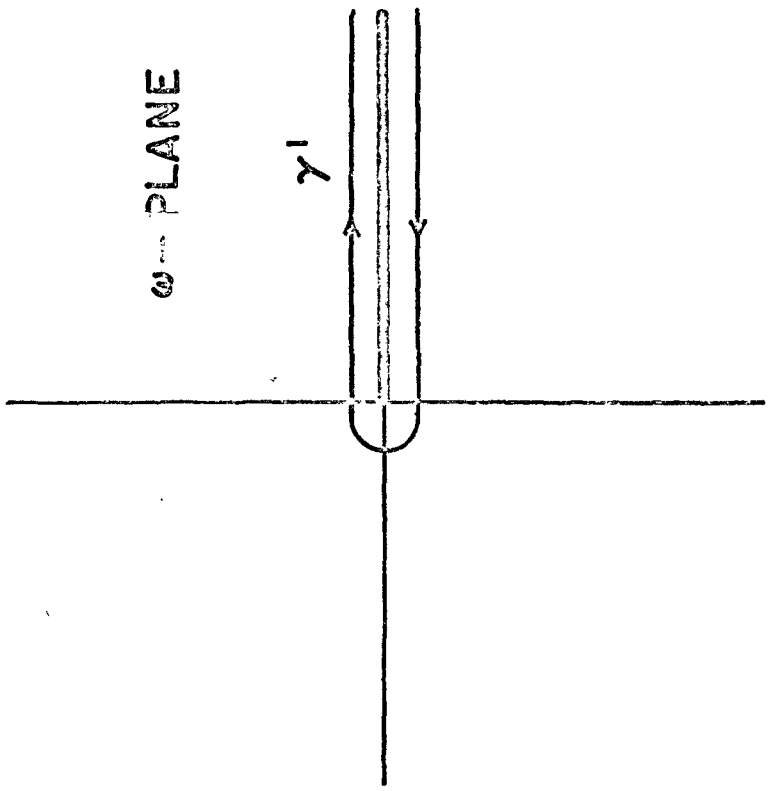


FIG. 3(b)

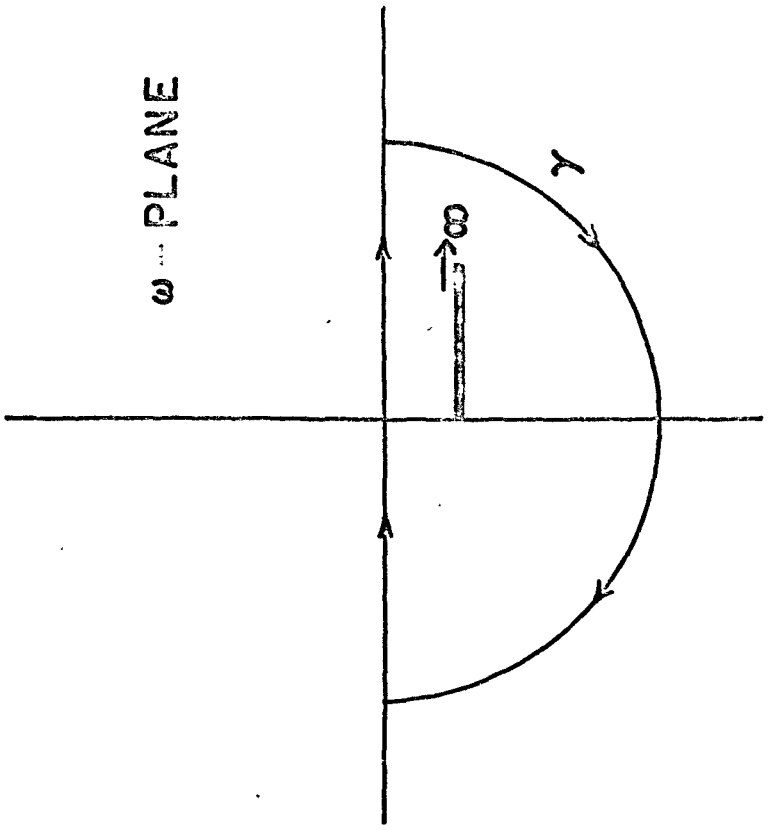


FIG. 3(a)

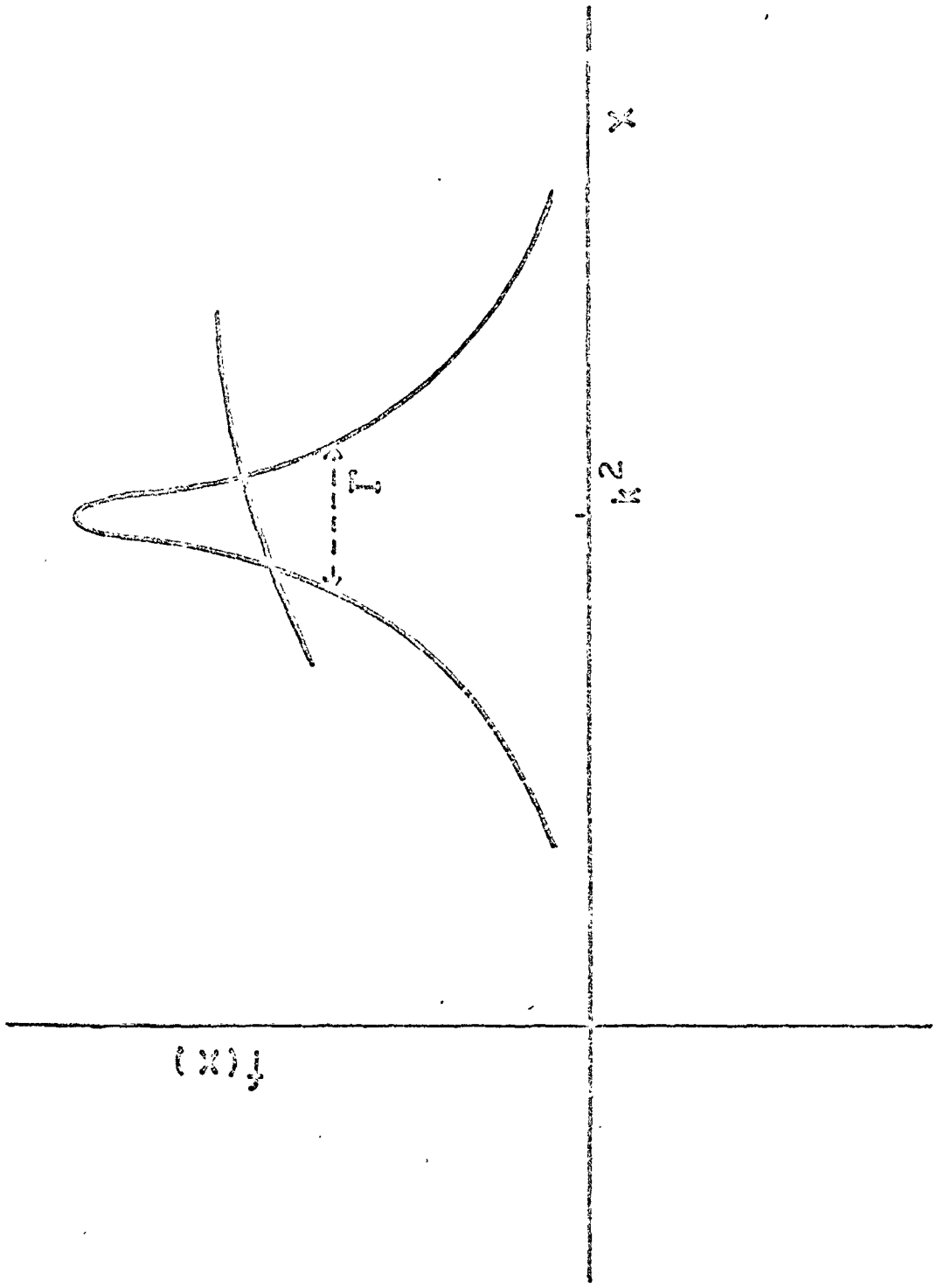
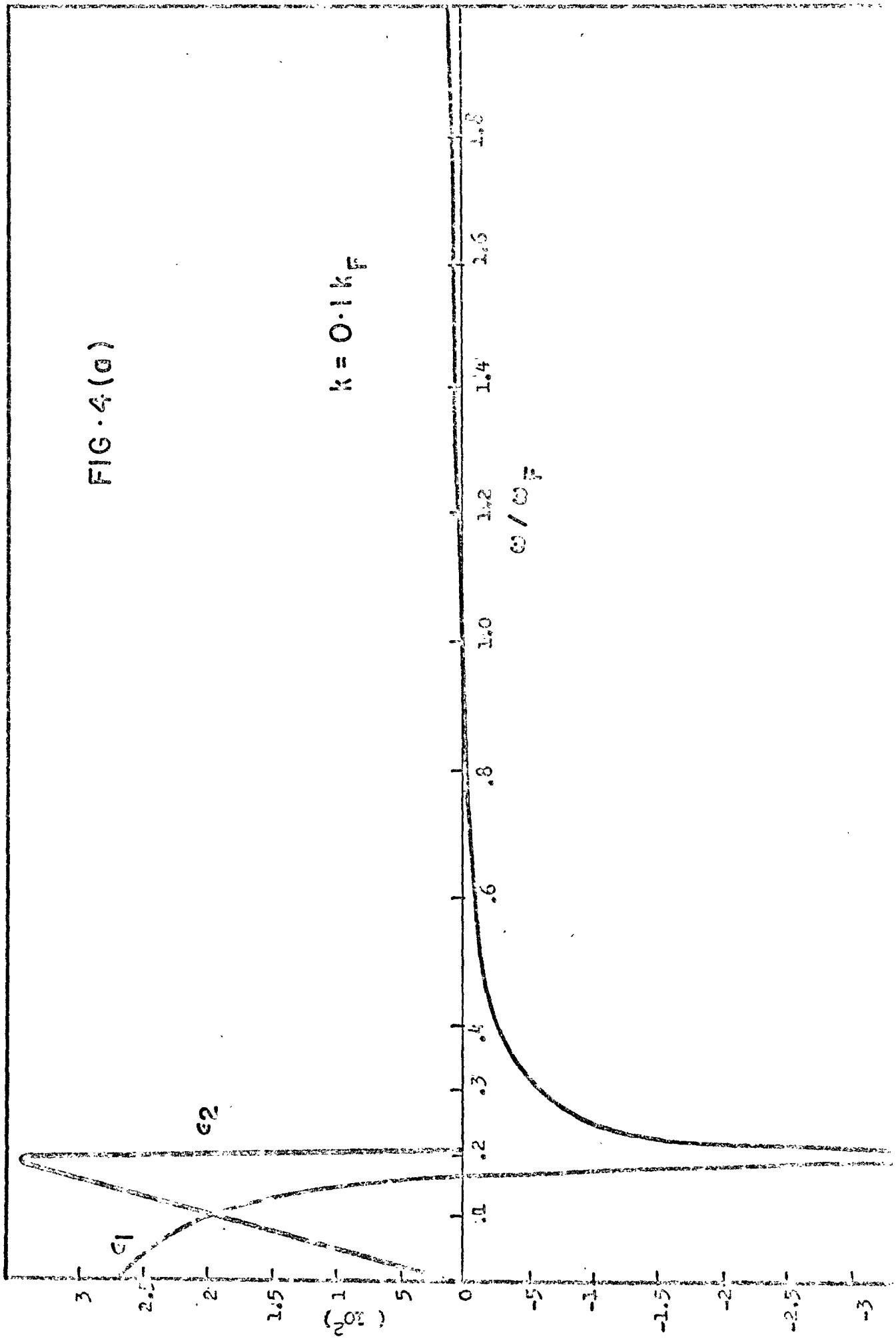


FIG. 3(c)


FIG·4(a)
k = 0·1 k_F
ε1
ε2
ω / ω_F
(2ω²)

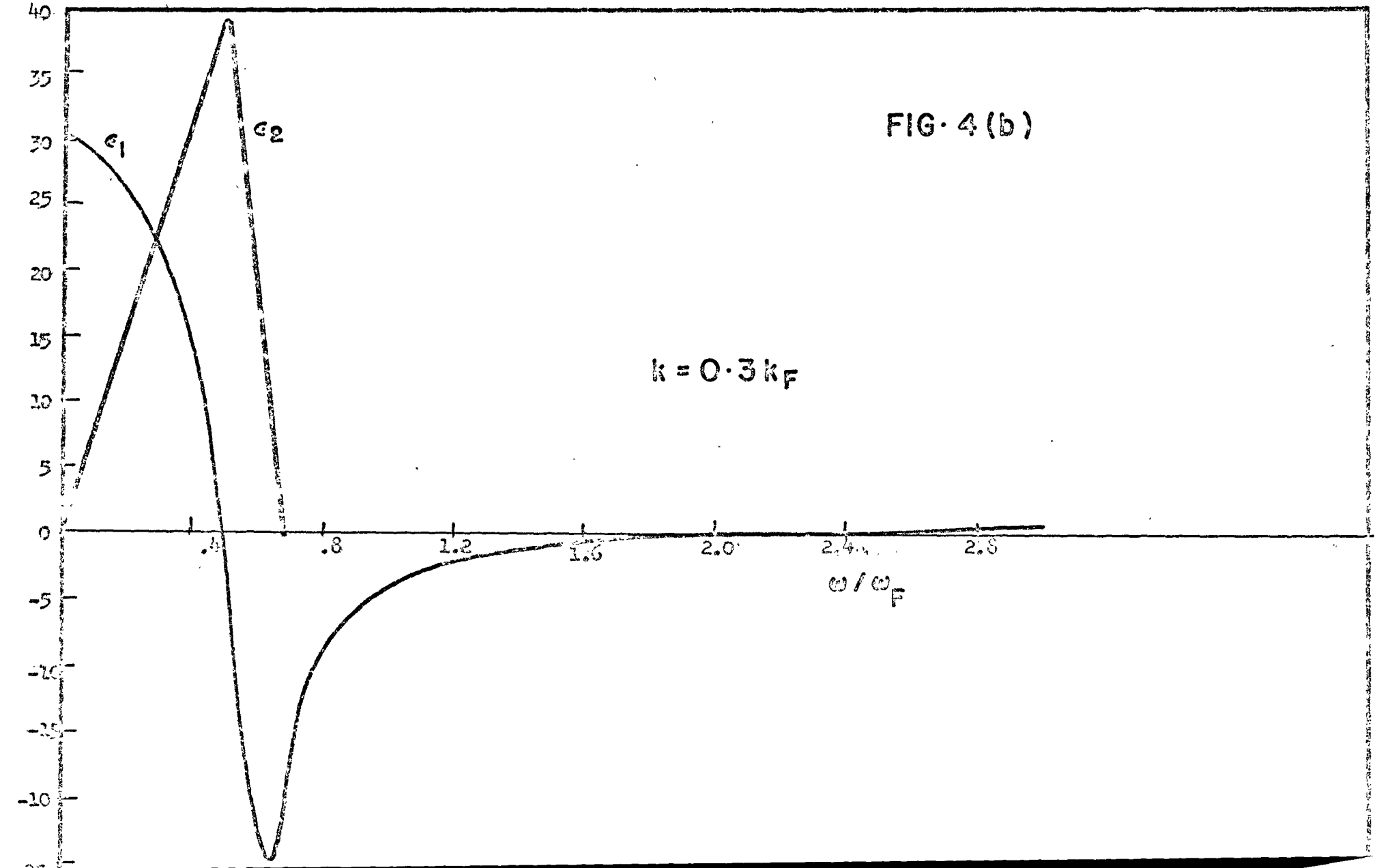

40
35
30
25
20
15
10
5
0
-5
-10
ϵ_1
ϵ_2
.4
.8
1.2
1.6
2.0
2.4
2.8
ω / ω_F
$k = 0 \cdot 3 k_F$

FIG. 4 (b)

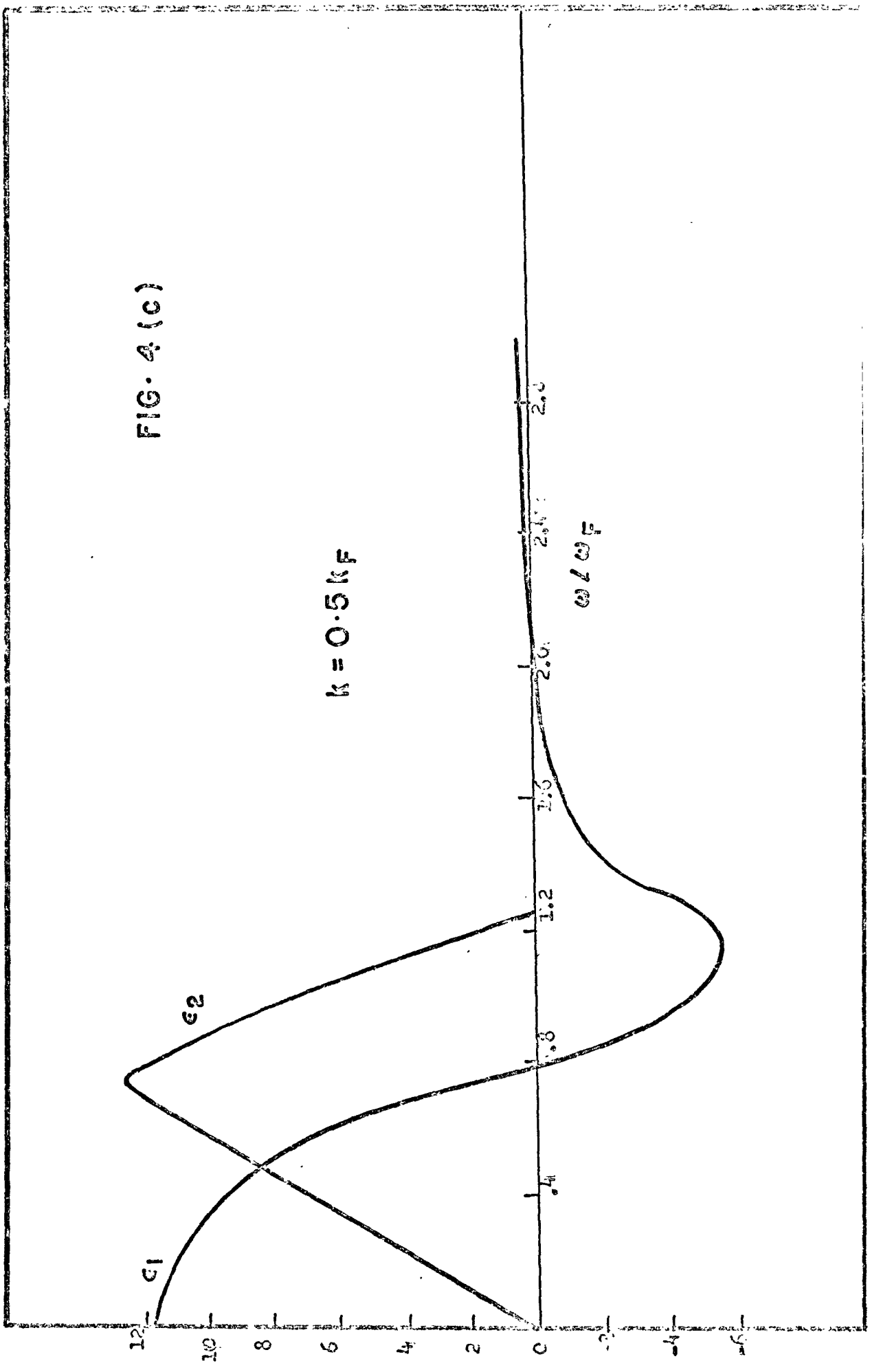


FIG. 4 (c)
k = 0.5 kF
ω / ωF
ε1
ε2
12
10
8
6
4
2
0
1.2
.8
.4

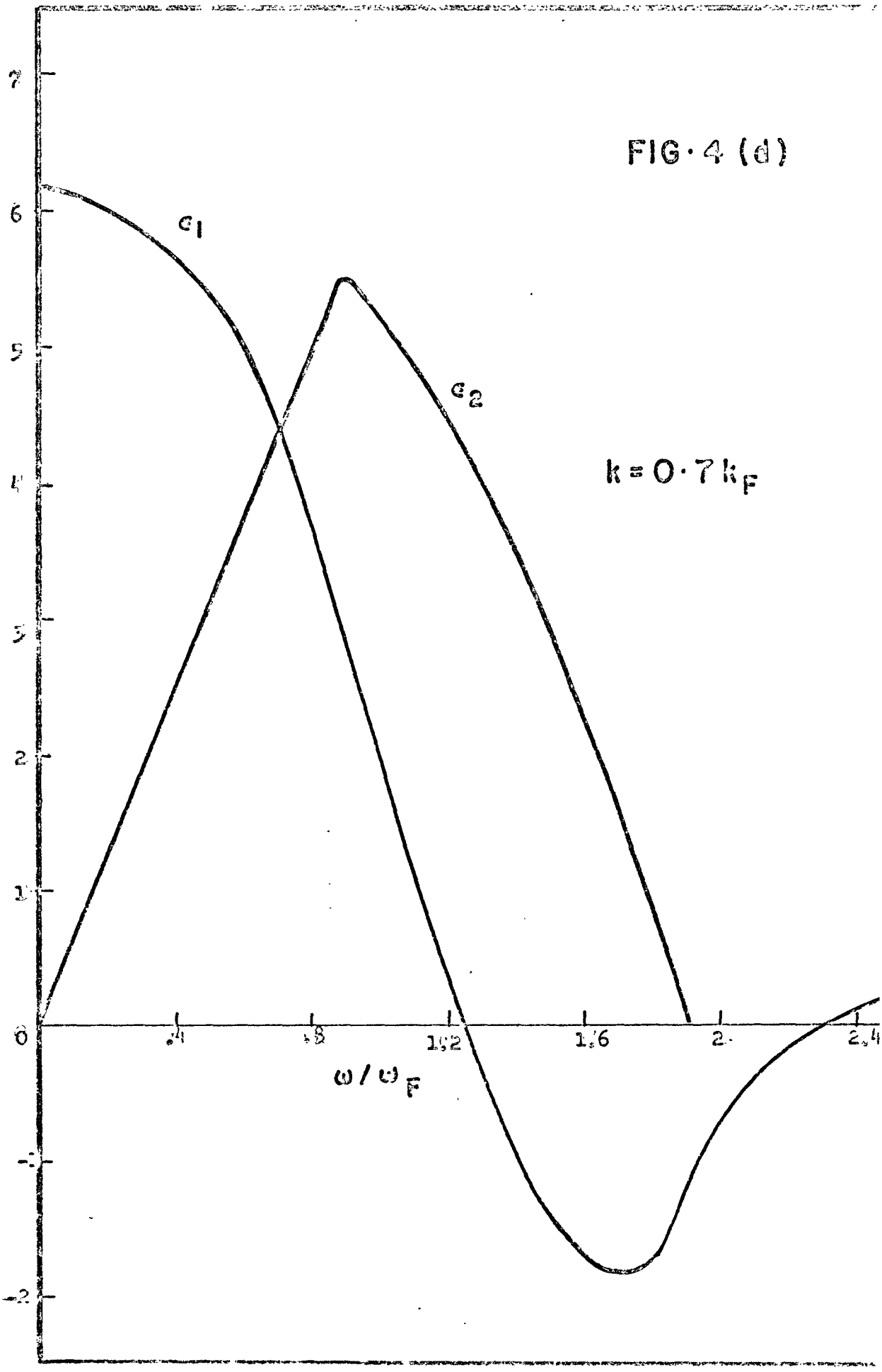
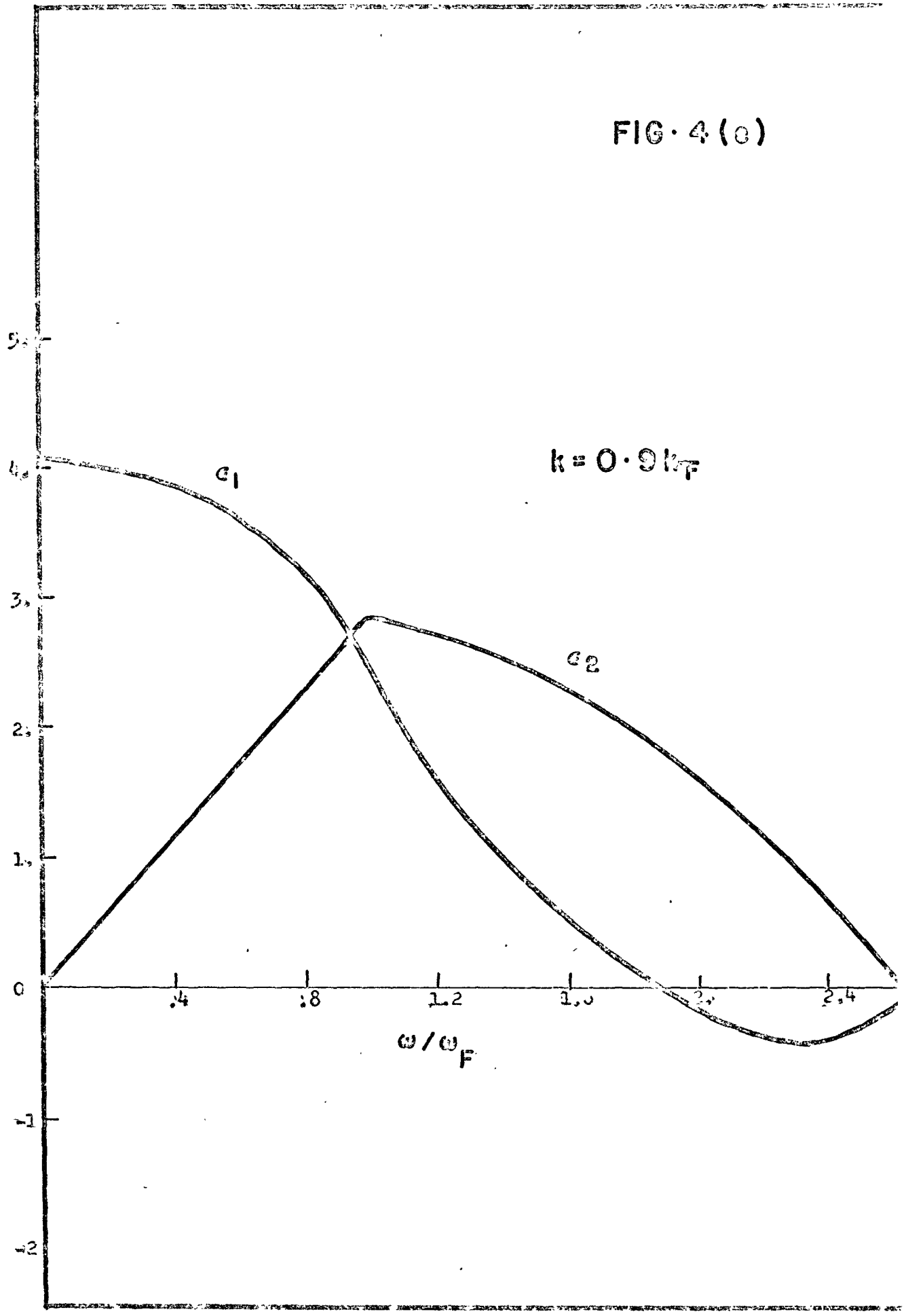
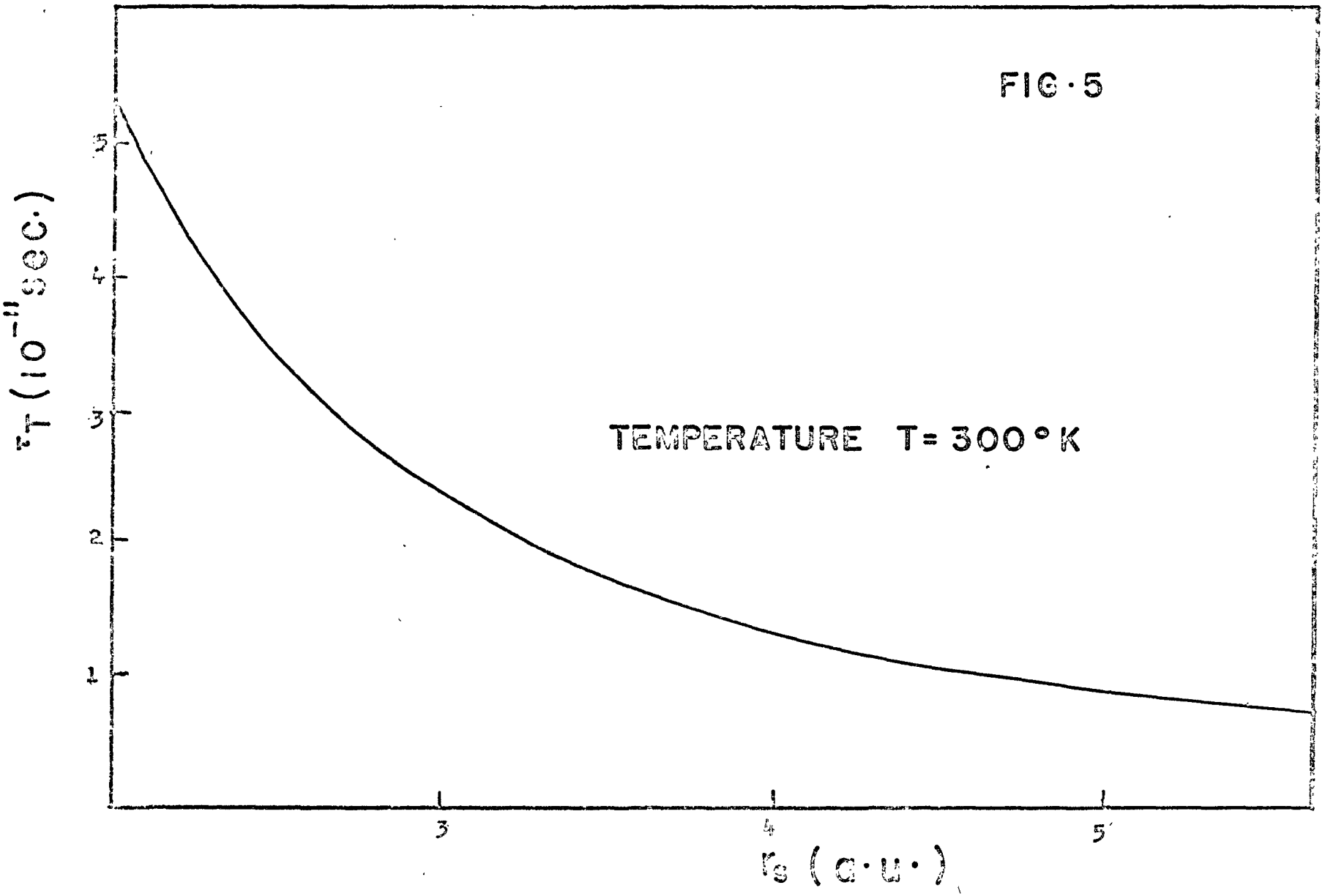

FIG·4 (d)
c_1
c_2
$k = 0{\cdot}7\, k_F$
7
6
5
4
3
2
1
0
-1
-2
.4
.8
1.2
1.6
2.
2.4
ω / ω_F

FIG · 4 (a)




FIG·5
TEMPERATURE T= 300°K
τ_T (10^{-11} sec.)
1
2
3
4
5
3
4
5
r_s (a·u·)

FIG·6

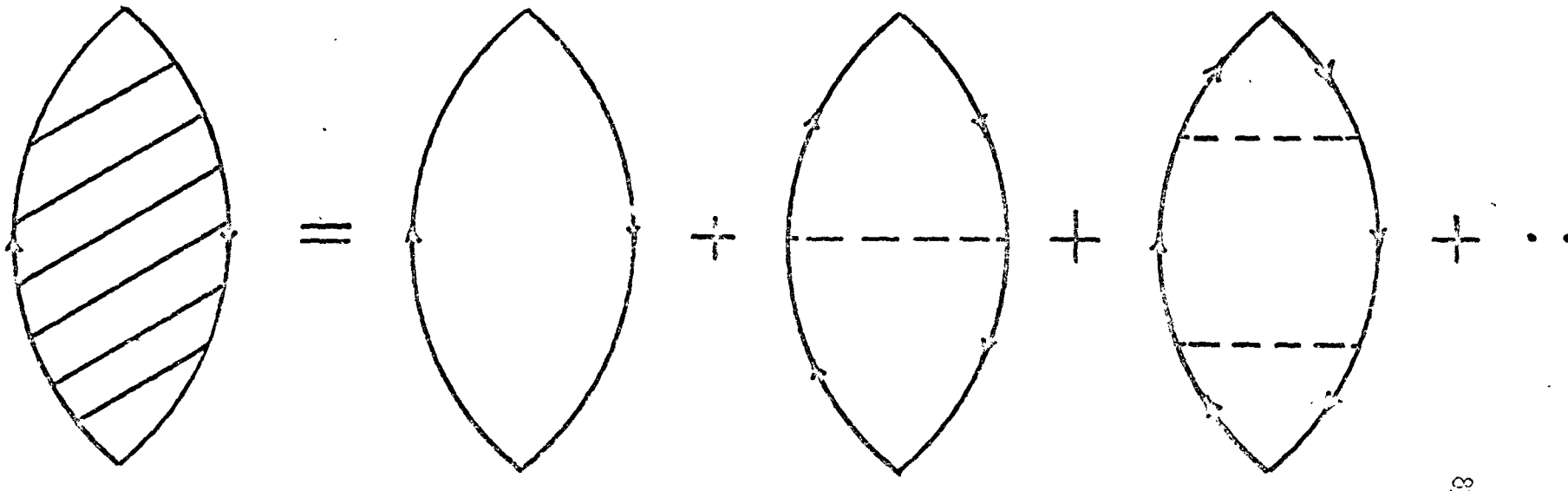


FIG. 7(a)

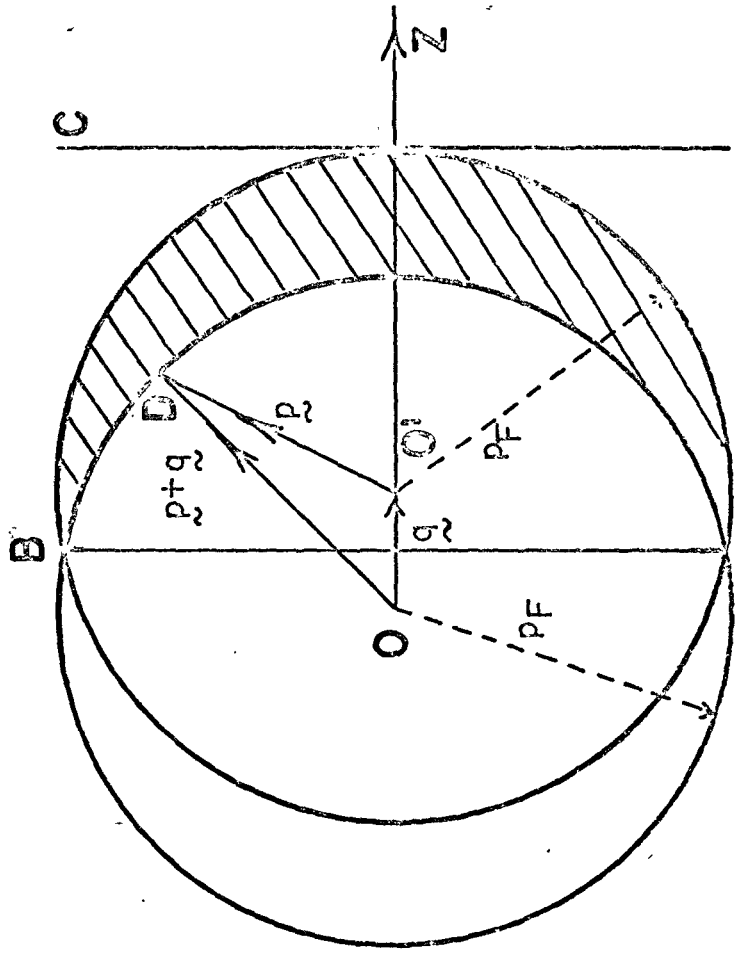


FIG. 7 (b)

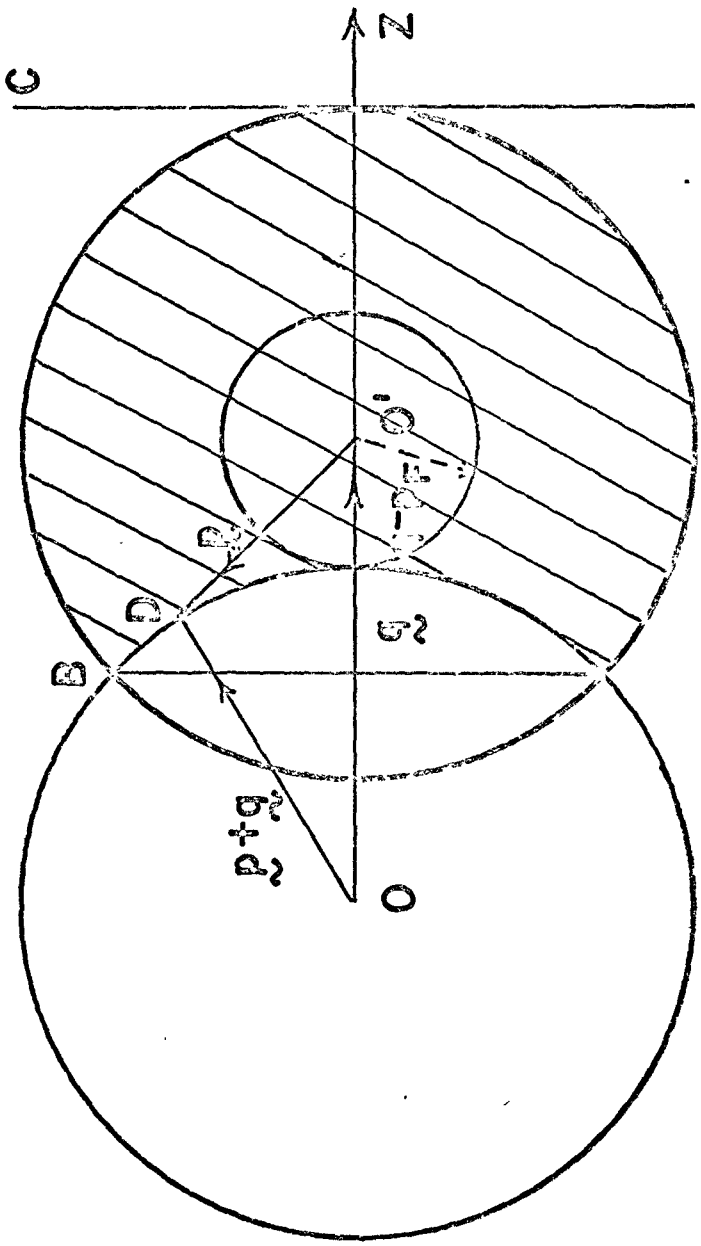


FIG. 7(c)

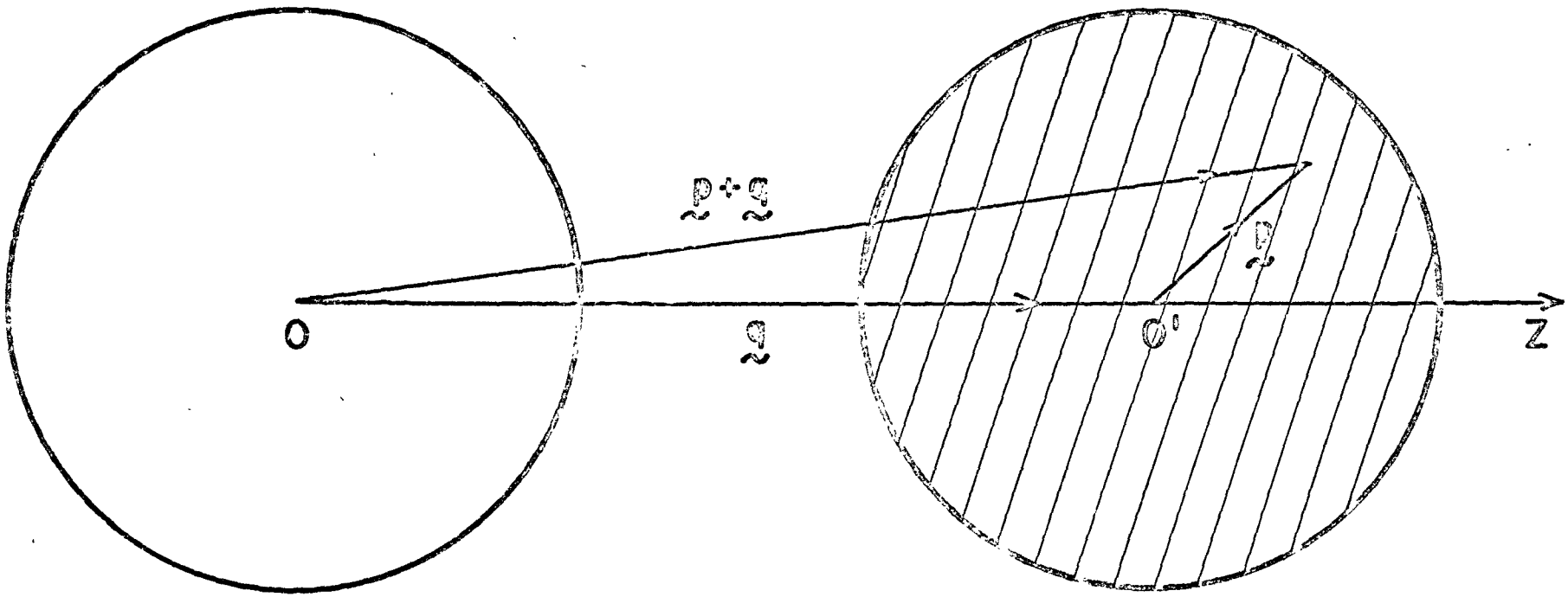


FIG. 7 (d)

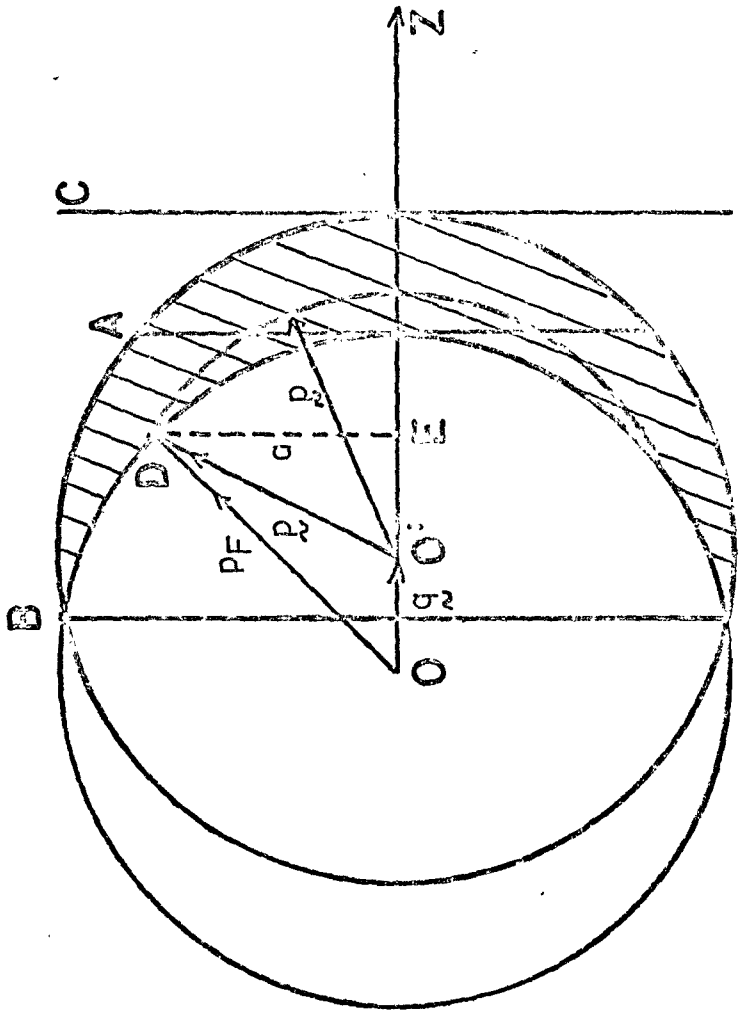


FIG. 7(e)

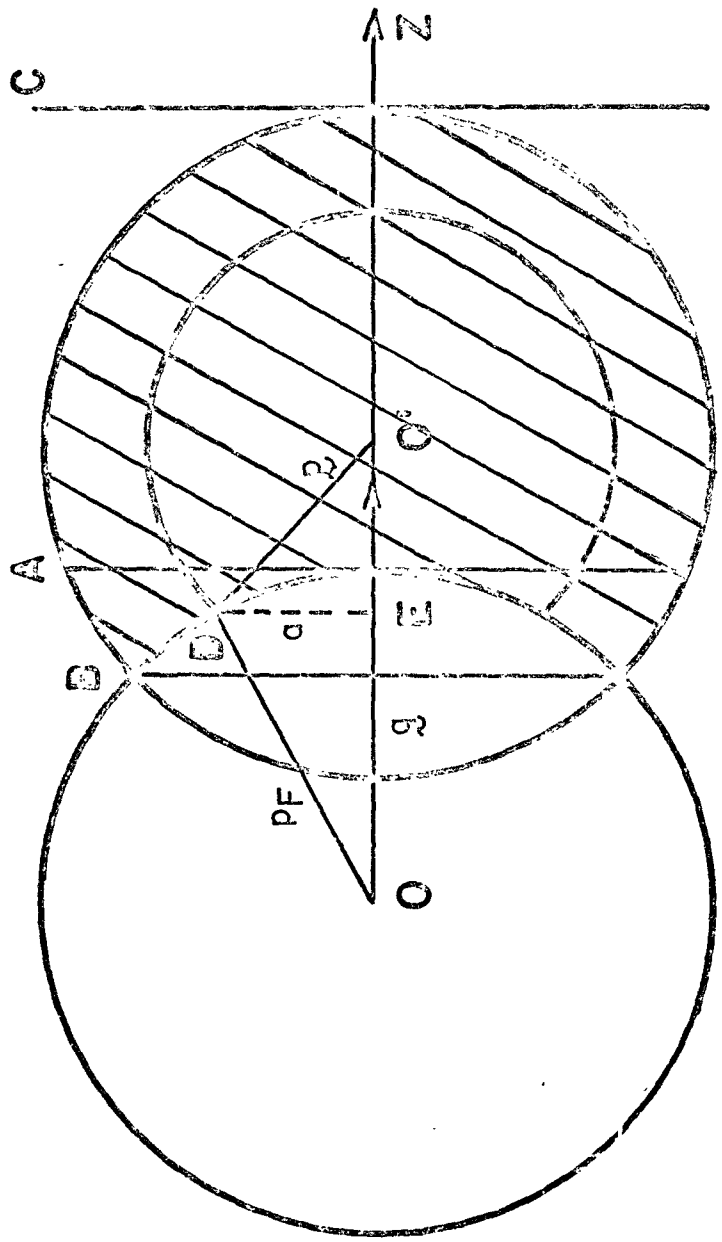


FIG · 7 (f)

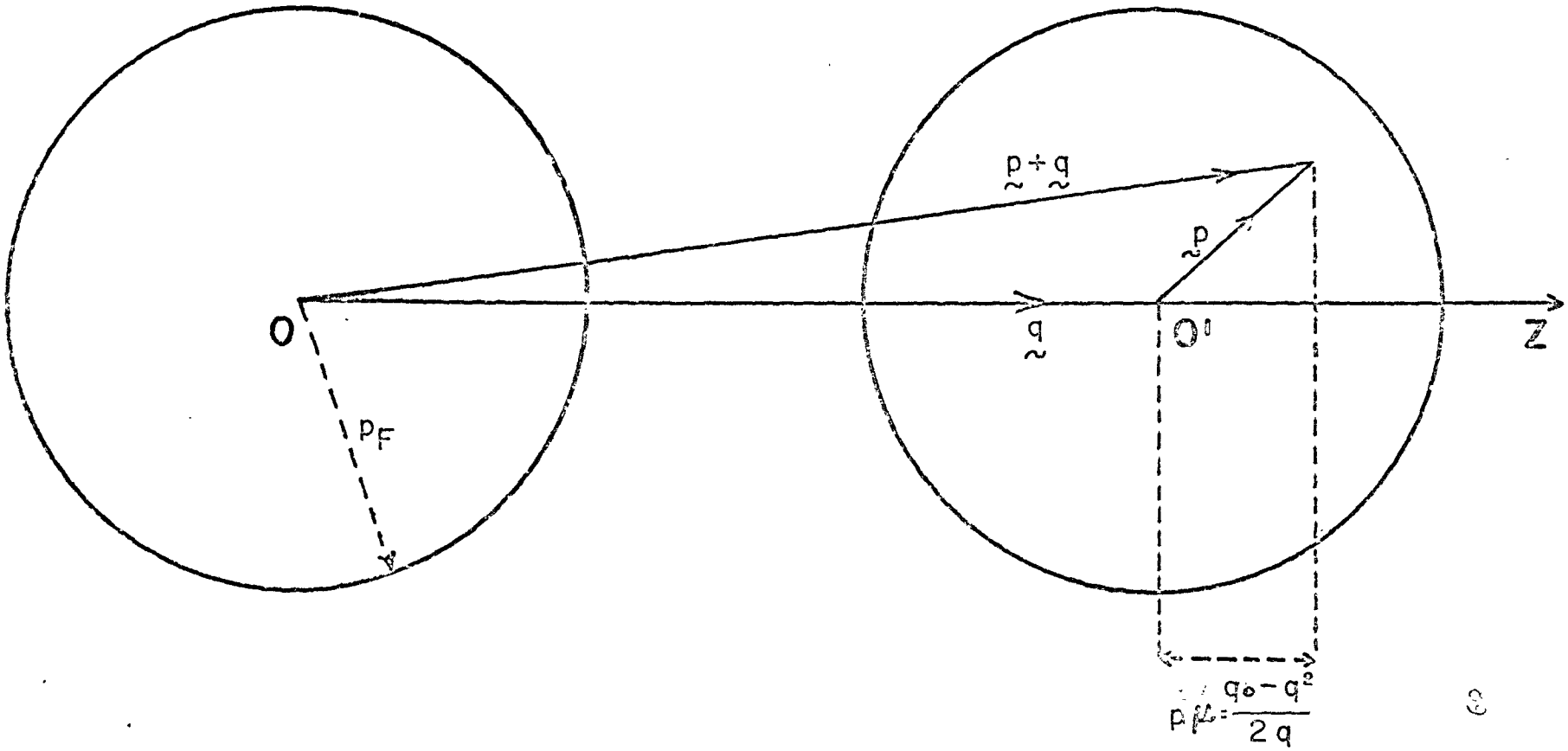

O
p_F
$\underset{\sim}{p}+\underset{\sim}{q}$
$\underset{\sim}{p}$
$\underset{\sim}{q}$
O'
Z
$p\mu = \frac{q_0 - q^2}{2q}$

TABLE 1

The peak width Γ (e.v.) of the integrand of equation (3.8), without the exponential, as a function of the positron energy (.1 e.v. - .01 e.v.) for values of r_s (2 - 6 in a. u.)

E(e.v.) / r_s(a.u.)	.10	.09	.08	.07	.06	.05	.04	.03	.02	.01
2.0	.00017	.00013	.00011	.00008	.00006	.00004	.00003	.000015	.000007	.000002
2.5	.00026	.00021	.00017	.00013	.00009	.00007	.00004	.000024	.000010	.000003
3.0	.00037	.00030	.00024	.00018	.00013	.00009	.00006	.000034	.000015	.000004
3.5	.00050	.00041	.00032	.00025	.00018	.00013	.00008	.000046	.000020	.000005
4.0	.00066	.00053	.00042	.00032	.00024	.00017	.00011	.000060	.000027	.000007
4.5	.00083	.00067	.00053	.00041	.00030	.00021	.00013	.000076	.000034	.000008
5.0	.00102	.00083	.00066	.00051	.00037	.00026	.00017	.000094	.000042	.000010
5.5	.00124	.00101	.00080	.00061	.00045	.00031	.00020	.000113	.000051	.000013
6.0	.00147	.00120	.00095	.00073	.00054	.00037	.00024	.000135	.000060	.000015