PHYSICAL REVIEW VOLUME 140, NUMBER 1A 4 OCTOBER 1965

Two Contributions to the Theory of Annihilation of Positrons in Metals. II. Effective Mass of the Positron

CHANCHAL K. MAJUMDAR*
Carnegie Institute of Technology, Pittsburgh, Pennsylvania

(Received 12 May 1965)

An experiment to measure the effective mass m_+^* of positrons in metals is discussed. We take advantage of the fact that there is a sharp break in the angular-correlation curve of the annihilation γ rays at the Fermi momentum. The experiment then consists in a study of the temperature dependence of the angular-correlation curve, to find how this break disappears with rise of temperature.

IN this paper, we shall present a detailed analysis of the temperature dependence of the angular-correlation curve of the γ rays due to positron annihilation in metals. This study resulted in a proposal to measure the effective mass of the positron in metals. The experimental analysis has been successfully carried out by Professor A. T. Stewart,[1] who finds, in sodium, the effective mass of the positron $m_+^*=(1.9\pm0.3)m$, where m is the electronic effective mass in sodium.

Theoretically, one expects an effective mass larger than unity, since the positron will occupy the lowest band, and all the energy denominators in the second-order perturbation theory are negative. This argument is completely analogous to one used to explain the effective mass in lithium, in contrast to other alkali metals, being larger than unity. The value of the effective mass m_+^* appears to have been first estimated by Dresselhaus[2] to be close to unity. Otherwise no attempt to calculate the effective mass from first principles has been made.

I. OPERATIONAL DEFINITION OF THE EFFECTIVE MASS

In some of his early experiments, Stewart[3] tried to take into account the effect of the momentum of the positron in analyzing his data on the angular correlation in metals, in solid as well as liquid phase. His procedure is easily adapted to provide an operational definition of the effective mass, m_+^*. Throughout our previous work, we have assumed that the positrons become thermalized in the solid and come to equilibrium at the same temperature as the solid itself. This is based on the detailed calculation of Lee-Whiting[4] on the thermalization time of positrons, which is found to be appreciably shorter than the lifetime, even at fairly low temperatures. Since the annihilation rate is practically velocity independent, the final distribution for low concentration of positrons can be taken to be a Maxwellian characteristic of the temperature T of the solid:

$$g(\mathbf{p})=[1/(2\pi m_+^*k_BT)^{3/2}]\exp[-\mathbf{p}^2/2m_+^*k_BT]. \quad (1.1)$$

k_B is the Boltzmann's constant. This equation defines the effective mass m_+^*. A similar definition is implicit in Stewart's work.

We have demonstrated in the previous paper[5] that for simple normal metals the angular correlation curve will manifest a sharp break at the Fermi momentum in the limit of zero temperature. At nonzero temperature, when the diffuseness of the Fermi surface due to electronic momenta is still negligible, the finite momentum of the positron will cause the intensity of the γ rays to rise at the Fermi momentum, above that expected at zero temperature. The rate of rise will be shown below to be proportional to $T^{1/2}$ and is quite different from that due to other effects, such as mean free path or thermal expansion which will be proportional to T or higher powers of T.

The order of magnitude of this effect is expected to be a few percent of the intensity at the center, and with the precision now available, it is easily measurable. However, the effect due purely to positrons is also accompanied by several other effects mentioned above and will have to be disentangled carefully.

We shall give below general theoretical formulas based entirely on the free-electron model. The work of the previous paper shows that it is not unjustified for normal metals. We analyze later the mean-free-path effect, thermal expansion, and finite resolution of the instrument. Studying the suitable conditions of the experiment, we discuss finally the relative merits of the metals available for study.

II. TEMPERATURE EFFECT OF POSITRON MOMENTUM

To calculate the probability that the γ rays have a momentum K_z in the Z direction, we first fold the momentum distribution of the electron, given by the usual Fermi function, with the distribution of the positron (1.1); this gives the probability $P(\mathbf{K})$ of total momentum $\mathbf{K}$, and then integrating over K_x, K_y we get

---

* Supported in part by National Science Foundation.

[1] A. T. Stewart and J. B. Shand, Bull. Am. Phys. Soc. **10**, 21 (1965).

[2] G. Dresselhaus, J. Phys. Chem. Solids **1**, 14 (1956).

[3] A. T. Stewart, J. H. Kusmiss, and R. H. March, Phys. Rev. **132**, 495 (1963).

[4] G. E. Lee-Whiting, Proc. Roy. Soc. **A212**, 362 (1952); Phys. Rev. **97**, 1557 (1955).

[5] C. K. Majumdar, preceding paper, Phys. Rev. **140**, A227 (1965).

for $P(K_z)$:

$$P(K_z)=\lambda\int\!\!\int_{-\infty}^{\infty} dK_x dK_y \int\!\!\int\!\!\int_{-\infty}^{\infty} \frac{dp_x dp_y dp_z}{(2\pi m_+^* k_B T)^{3/2}} \frac{\exp[-(\mathbf{K}-\mathbf{p})^2/2m_+^* k_B T]}{\exp[(E_{\mathbf{p}}-\mu)/k_B T]+1}. \tag{2.1}$$

μ is the Fermi energy. λ is a constant depending on experimental conditions, source strength for instance.

Let us assume that we have a spherical Fermi surface. The energy surfaces are also spherical, so that $E_{\mathbf{p}}=\mathbf{p}^2/2m$, m being the electronic effective mass. Since the integrals in (2.1) are obviously convergent, we can change the order of integrations. First we perform the integrations over K_x, K_y and then over p_x, p_y by introducing cylindrical polar coordinates. This gives the exact formula:

$$P(K_z)=\lambda(2\pi k_B T)^{1/2}\frac{m}{m_+^{*1/2}}\int_{-\infty}^{\infty} dp_z \exp[-(K_z-p_z)^2/2m_+^* k_B T] \ln\left[1+\exp\left(\frac{\mu}{k_B T}-\frac{p_z^2}{2mk_B T}\right)\right]. \tag{2.2}$$

To eliminate the constant λ, we will always compare the intensities at two points. The obvious choices are $K_z=0$ and $K_z=k_F$. At $K_z=0$, the geometry of the apparatus is well defined, and high precision is possible, while at k_F the effect due to positron momenta will be maximum. For temperatures low compared with the Fermi temperature T_F of the electrons, we get

$$P(K_z=0)=\lambda\pi k_F^2[1-\tfrac{1}{2}(m_+^*/m)\cdot(T/T_F)]+\cdots,$$

$$P(K_z=k_F)=\lambda k_F(2\pi m_+^* k_B T)^{1/2}-\tfrac{1}{2}\lambda\pi m_+^* k_B T+\frac{\lambda\pi}{12}\frac{(m\pi k_B T)^{3/2}}{m_+^{*1/2}\mu^{1/2}}+\cdots,$$

and

$$\frac{P(k_F)}{P(0)}=\frac{1}{\pi^{1/2}}\left(\frac{m_+^* T}{mT_F}\right)^{1/2}-\frac{1}{4}\frac{Tm_+^*}{T_F m}+\frac{1}{2\pi^{1/2}}\left(\frac{m_+^* T}{mT_F}\right)^{3/2}+\frac{\pi^{3/2}}{24}\left(\frac{m}{m_+^*}\right)^{1/2}\left(\frac{T}{T_F}\right)^{3/2}+\cdots. \tag{2.3}$$

A similar calculation on an ellipsoidal Fermi surface, described in Appendix A, gives

$$\frac{P(k_F)}{P(0)}=\frac{1}{\pi^{1/2}}\left(\frac{m_+^* T}{m_3 T_F}\right)^{1/2}-\frac{1}{4}\frac{m_+^* T}{m_3 T_F}+\frac{1}{2\pi^{1/2}}\left(\frac{m_+^* T}{m_3 T_F}\right)^{3/2}+\frac{\pi^{3/2}}{24}\left(\frac{m_3}{m_+^*}\right)^{1/2}\left(\frac{T}{T_F}\right)^{3/2}+\cdots. \tag{2.4}$$

m_3 is the effective mass in the Z direction. For metals, $T/T_F\sim 1/50$ to $1/100$. Hence the intensity at the Fermi momentum will be 5 to 10% of that at the center.

III. EXTRANEOUS EFFECTS

We shall now estimate the effect of finite mean free path and thermal expansion on the observed correlation curve. To study the first, we consider the momentum distribution of the free-electron gas in the presence of static impurities. This is given by (see Appendix B)

$$n_{\mathbf{K}}=\int_{-\infty}^{\infty}\frac{d\omega}{e^{\beta\omega}+1}\frac{1}{\pi}\frac{\Gamma(\mathbf{K},\omega)}{(\omega-\epsilon_{\mathbf{K}}+\mu)^2+\Gamma^2(\mathbf{K},\omega)}. \tag{3.1}$$

The observed γ-ray curve will be

$$P_1(K_z)=\lambda\int\!\!\int_{-\infty}^{\infty} dK_x dK_y n_{\mathbf{K}}=\lambda\int\!\!\int_{-\infty}^{\infty} dK_x dK_y \int_{-\infty}^{\infty}\frac{d\omega}{e^{\beta\omega}+1}\frac{\Gamma(\mathbf{K},\omega)}{\pi[(\omega-\epsilon_{\mathbf{K}}+\mu)^2+\Gamma^2(\mathbf{K},\omega)]}. \tag{3.2}$$

We know the mean-free-path effect will be maximum at $\omega=0$ which corresponds to the Fermi energy, and $\Gamma(\mathbf{K},0)$ has a maximum at k_F. Hence we shall put $\Gamma(\mathbf{K},\omega)=\Gamma(k_F,0)$ and treat it as a number only. This probably overestimates the mean-free-path effect. This gives

$$P_1(K_z)=\lambda\left[2m\Gamma(k_F,0)+2\pi mk_B T\ln\left\{1+\exp\left[\frac{1}{k_B T}\left(\mu-\frac{K_z^2}{2m}\right)\right]\right\}\right].$$

TABLE I. Mean free paths calculated from Eq. (3.5) and conductivity.

T°K	l(3.5) (cm)	l_{cond} (cm)
200	17.4×10^{-8}	(K) 260×10^{-8} (320°K)
400	12.4×10^{-8}	(Ca) 86×10^{-8} (750°K)
900	8.2×10^{-8}	(Na) 220×10^{-8} (370°K)
1600	6.2×10^{-8}	(Li) 75×10^{-8} (450°K)

So

$$\begin{aligned} P_1(k_F) &= 2m\lambda\Gamma(k_F,0)+2\pi m\lambda k_B T\ln 2\,,\\ P_1(0) &= \lambda\pi k_F{}^2+2m\lambda\Gamma(k_F,0)\,. \end{aligned} \tag{3.3}$$

Introducing a mean free path l and the Fermi velocity u_F of the electron, we get

$$P_1(k_F)/P_1(0)=hu_F/\pi k_B T_F l+(mT/T_F)\ln 2\,. \tag{3.4}$$

This mean free path is different from that measured via conductivity and is expected to be slightly smaller. Equating the term involving the mean free path to the leading term in Eq. (2.3), one obtains

$$\bar{l}=h(2/\pi m_+{}^* k_B T)^{1/2}\,. \tag{3.5}$$

Assuming $m_+{}^*$ to be one, the values of $\bar{l}$ are given in Table I. The conductivity mean free path can be calculated from

$$l_{\text{cond}}=9.79\times10^{-25}\sigma r_s{}^2\text{ cm}\,,$$

where the conductivity σ is in electrostatic units and r_s is the usual dimensionless parameter characterizing metals. These values of l_{cond} are also given in Table I for some materials of interest. For good conductors, the conductivity mean free paths are 10 to 15 times larger than that calculated from (3.5), and it is expected that the relevant mean free path is also appreciably larger. Hence the effect is smaller than the positron effect at the temperatures of interest. It is also clear that this mean-free-path effect is, at most, directly proportional to temperature. Thus the entire effect is in higher powers of temperature, as compared with the positron effect.

The effect of thermal expansion is much larger, but can be quantitatively accounted for, by knowing the thermal expansion coefficient for the material, provided the Fermi surface maintains its shape. For this we require the Fermi surface be spherical. In that case, the volume expansion of the material, assumed isotropic, will simply cause the Fermi momentum to decrease. In the angular-correlation curve, the intensity at the center will increase. This can be calculated, as the area under the curve is just proportional to the number of positrons injected into the system, which is assumed constant. The area under the curve is $\frac{2}{3}hk_F$, where h is the central maximum.

At temperature T, the Fermi momentum is

$$k_F(T)=k_F(0)-k_F(0)\int_0^T\alpha(T')dT'\,,$$

(α is the linear expansion coefficient). Since $hk_F=$ constant, the change in the central maximum, δh, is

$$\frac{\delta h}{h}=-\frac{\delta k_F}{k_F(0)}=\int_0^T\alpha(T')dT'\,.$$

Hence

$$h(T)=h(0)+h(0)\int_0^T\alpha(T')dT'\,. \tag{3.6}$$

As the Fermi surface maintains its shape, the parabola at temperature T is represented by

$$P_2(K_z)=h(T)\{1-[K_z{}^2/k_F(T)^2]\}\,. \tag{3.7}$$

Since the thermal expansion coefficient is experimentally measurable, we can determine the form $P_2(K_z)$ from (3.7) and find the necessary correction. It is seen easily that at the true Fermi momentum for 0°K there is no correction at all. However, since we always compare the intensity at k_F with that at the center, the rise at the center will contribute a diminution in the ratio

$$\left\{h(0)\Big/h(0)\left[1+\int_0^T\alpha(T')dT'\right]\right\}-1$$
$$=-\int_0^T\alpha(T')dT'\,. \tag{3.8}$$

Collecting all the terms up to order T/T_F from (2.3), (3.4), and (3.8), we obtain the complete theoretical expression

$$\frac{P(k_F)}{P(0)}=\frac{1}{\pi^{1/2}}\left(\frac{m_+{}^*T}{mT_F}\right)^{1/2}-\frac{1}{4}\frac{m_+{}^*T}{mT_F}$$
$$+\frac{hu_F}{\pi k_B T_F l}+\frac{mT}{T_F}\ln 2-\int_0^T\alpha(T')dT'\,. \tag{3.9}$$

At temperatures below the Debye temperature, the last term will be small, and the mean-free-path effect will also decrease as thermal fluctuations die out. Around the Debye temperature one expects to see an almost pure $T^{1/2}$ behavior.

The major complication in the experiment is due to, as always, finite resolution. If the resolution functions were perfectly known, it would be possible to eliminate its effect, at least in principle, by the following procedure:

Let $I(K)$ denote the observed curve and $I_0(K)$ that in the limit of perfect resolution. Clearly,

$$I(K)=\int_{-\infty}^{\infty}R(K-p)I_0(p)dp\,, \tag{3.10}$$

where the kernel $R(K-p)$ is due to finite resolution; this is approximately Gaussian in form. The formal solution to (3.10) is

$$I_0(K)=\frac{1}{\pi}\int_0^{\infty}\frac{I(q)}{R(q)}\cos qKdq\,, \tag{3.11}$$

where $I(q)$, $R(q)$ are the Fourier transforms:

$$I(q)=\left(\frac{2}{\pi}\right)^{1/2}\int_0^\infty I(p)\cos qp\,dp\,,$$

$$R(q)=\left(\frac{2}{\pi}\right)^{1/2}\int_0^\infty R(p)\cos qp\,dp\,.$$

Since the experimental curves and the resolution function are well behaved, the transforms obviously exist.

Unfortunately, such a procedure is not warranted because of imprecise knowledge of resolution. As a consequence, one may encounter a number of difficulties. First, the true Fermi momentum used in (3.9) will not be exactly known, even from low-temperature data. This is not very serious, and one can always determine k_F by other experimental methods to better than one percent accuracy. Secondly, the thermal-expansion correction becomes somewhat uncertain. Let us recall that the effect at the Fermi momentum of 0°K vanished. However, quite close to it, at the Fermi momentum of the temperature of the experiment, the correction has a maximum. Because of finite resolution one should consider this carefully. Of course, thermal expansion has a different temperature dependence and is important only at high temperature. Also the terms linear in T have different signs and will tend to cancel each other. It is imperative to select out the $T^{1/2}$ behavior.

The experimental data can be represented by the formula

$$P(k_F)/P(0)=\Delta=c+aT^{1/2}+bT\,. \qquad (3.12)$$

The constant comes from finite resolution. If one now plots $\Delta/T^{1/2}$ against $T^{1/2}$, one will get a curve that will be a straight line above and around the Debye temperature. At very low temperature, owing to finite resolution, the curve will wander off to infinity; but the intercept of the straight line when extrapolated to $T=0$°K will give the effective mass m_+^*.

IV. CHOICE OF THE METAL

It is quite clear that the metal should satisfy the following requirements:

(i) To avoid complications in thermal expansion the Fermi surface should be nearly spherical.

(ii) It should have high T_M/T_F and Θ_D/T_F, in order to maximize the positron effect, and minimize the thermal-expansion problem (the melting point is denoted by T_M and the Debye temperature by Θ_D). The difference $(T_M-\Theta_D)$ should be appreciable so that one gets enough experimental points for drawing the straight line of Eq. (3.12).

(iii) It should be a good conductor, even at high temperature, and fulfill the requirements of Table I.

The first requirement restricts us to "simple" metals. In Table II, we present the relevant parameters T_F/T_M and Θ_D/T_F for most simple metals; we regard all electrons outside the closed atomic shell as free, so that alkali metals are monovalent, aluminium is trivalent, and lead is quadrivalent. The smooth variation of r_s, T_F/T_M, and Θ_D/T_F in each column of the periodic table is indeed remarkable.

TABLE II. Melting point T_M, Debye temperature Θ_D, and Fermi temperature T_F of materials available for m_+^* experiment.

Metal	r_s	Fermi temperature T_F (°K)	Melting point T_M (°K)	$\frac{T_F}{T_M}$	Debye temperature Θ_D (°K)	Θ_D/T_F
Li	3.27	5.49×10^4	459	120	363	0.62×10^{-2}
Na	3.97	3.70×10^4	371	100	150	0.41×10^{-2}
K	4.95	2.39×10^4	337	71	100	0.42×10^{-2}
Rb	5.30	2.09×10^4	312	67	58	0.28×10^{-2}
Cs	5.71	1.80×10^4	301	60	42	0.23×10^{-2}
Be	1.86	1.69×10^5	1557	109	1160	0.68×10^{-2}
Mg	2.65	8.34×10^4	923	90	290	0.35×10^{-2}
Ca	3.25	5.54×10^4	1124	49	230	0.42×10^{-2}
Sr	3.55	4.64×10^4	1044	44	171	0.37×10^{-2}
Ba	3.71	4.26×10^4	1123	38	113	0.27×10^{-2}
Ra	3.92	3.81×10^4	1233	31	···	···
Al	2.08	1.35×10^5	932	145	390	0.29×10^{-2}
Ga	2.19	1.22×10^5	303	405	125	0.10×10^{-2}
In	2.41	1.01×10^5	429	235	106	0.11×10^{-2}
Tl	2.48	9.50×10^4	577	165	100	0.11×10^{-2}
Si	2.00	1.47×10^5(?)	1687	87	650	0.44×10^{-2}
Ge	2.08	1.35×10^5(?)	1233	110	290	0.21×10^{-2}
Sn	2.21	1.20×10^5	505	238	260	0.22×10^{-2}
Pb	2.30	1.11×10^5	600	185	88	0.08×10^{-2}
Cu	2.67	8.22×10^4	1356	61	330	0.40×10^{-2}
Ag	3.01	6.45×10^4	1234	52	213	0.33×10^{-2}
Au	3.01	6.48×10^4	1336	49	170	0.26×10^{-2}
Zn	2.30	1.11×10^5	692	160	250	0.23×10^{-2}
Cd	2.59	8.72×10^4	594	147	172	0.20×10^{-2}
Hg	2.70	8.03×10^4	234	343	80	0.10×10^{-2}

As mentioned previously, Stewart[1] has carried out the experiment on sodium. Looking at Table II, we conclude that other suitable materials are potassium, lithium, and calcium. Calcium has an extremely favorable $T_F/T_M=49$, but it has a phase transition (fcc to bcc) at 740°K, and at that temperature $T_F/T_{\text{tr}}=73$, about the same as in potassium. We would like to point out several facts which may be of some consequence in experiments with these metals.

The Fermi surface of potassium is known to be almost spherical,[6] as in sodium, and it is a good conductor. However, it is a very soft metal, and the Fermi surface is easily distorted under stress. It is highly reactive and difficult to work with. The thermal expansion coefficient appears not to have been investigated thoroughly; but extensive specific-heat data exist,[7] and one can get the relevant information by using Grüneisen's law, the one known point around room temperature for expansion coefficient serving as reference point. Recently, there have also been suggestions that the ground state of potassium has strong pair correlations.[8,9] It

---

[6] M. H. Cohen and V. Heine, Advan. Phys. 7, 395 (1958).

[7] L. M. Roberts, Proc. Phys. Soc. 70, 744 (1957); C. A. Krier, R. S. Craig, and W. E. Wallace, J. Phys. Chem. 61, 522 (1957).

[8] M. H. Cohen and J. C. Phillips, Phys. Rev. Letters 12, 662 (1964).

[9] A. W. Overhauser, Phys. Rev. Letters 13, 190 (1964).

may be pointed out, however, that in both the theories of Cohen and Phillips[8] and of Overhauser[9] the discontinuity in momentum distribution persists, and thus a Fermi surface exists, though it may be shifted in certain crystal directions in the Overhauser case. This means, according to our previous paper, that a sharp break will be found in the angular-correlation curve and the experiment for m_+^* is feasible.

Calcium has a lower expansion coefficient and its conductivity and expansion coefficient are known. The Fermi surface has been constructed theoretically by W. Harrison[10]; and although it follows the free-electron sphere fairly well, there are contacts with zone boundaries in several directions. Its free-electron character cannot therefore be said to be ideal.

Lithium has anisotropies in the Fermi surface, in particular the question of contact with the zone boundary in the $\langle 110\rangle$ direction has not yet been completely cleared up experimentally. The difference $(T_M-\Theta_D)$ is also very short, although Θ_D/T_F is comfortably high.

It would be quite interesting to extend the positron effective-mass measurements to these materials. Of course, a major theoretical problem that remains to be solved is a calculation of m_+^* from first principles.

ACKNOWLEDGMENTS

The work was carried out in the University of California at La Jolla in partial fulfilment of the requirements of the Ph.D. degree, and supported by the Office of Naval Research. I would like to thank Professor Walter Kohn for suggesting the problem and for many discussions.

APPENDIX A

We shall here outline the calculation of Eq. (2.4) for ellipsoidal energy surfaces. The Fermi surface is described by

$$K_x^2/2m_1+K_y^2/2m_3+K_z^2/2m_3=\mu\,, \tag{A1}$$

where μ is the Fermi energy. The observed momentum distribution, when the z axis of observation coincides with the third principal axis of the Fermi surface, is

$$P(K_z)=\int_{-\infty}^{\infty}dK_xdK_y\int_{-\infty}^{\infty}d\mathbf{p}\frac{\exp[-(\mathbf{K}-\mathbf{p})^2/2m_+^*k_BT]}{(2\pi m_+^*k_BT)^{3/2}\left\{\exp\left[\left(\dfrac{p_x^2}{2m_1}+\dfrac{p_y^2}{2m_2}+\dfrac{p_z^2}{2m_3}-\mu\right)\Big/k_BT\right]+1\right\}}\,. \tag{A2}$$

We perform the K_x, K_y integrations first and introduce reduced coordinates

$$p_1=p_x/(2m_1)^{1/2},\quad p_2=p_y/(2m_2)^{1/2},\quad p_3=p_z/(2m_3)^{1/2}. \tag{A3}$$

We get, after carrying out the p_1, p_2 integrations,

$$P(K_z)=\left(\frac{4\pi k_BTm_1m_2m_3}{m_+^*}\right)^{1/2}\int_{-\infty}^{\infty}dp_3\exp\{-[K_z-(2m_3)^{1/2}p_3]^2/2m_+^*k_BT\}\ln[1+\exp\{(\mu-p_3^2)/k_BT\}]. \tag{A4}$$

This formula is exact. For further evaluation, we have to proceed numerically or make approximations.

Special Cases

i. $K_z=0$. We have

$$P(0)=\left(\frac{4\pi k_BTm_1m_2m_3}{m_+^*}\right)^{1/2}\int_{-\infty}^{\infty}dp_3\exp\left[-\frac{m_3p_3^2}{m_+^*k_BT}\right]\ln\left[1+\exp\left(\frac{\mu-p_3^2}{k_BT}\right)\right]. \tag{A5}$$

For low temperatures, $\mu\gg k_BT$ and

$$\ln\{1+\exp[(\mu-p_3^2)/k_BT]\}\simeq(\mu-p_3^2)/k_BT. \tag{A6}$$

The error comes mostly from near $\mu\simeq p_3^2$, but the Gaussian factor multiplying the logarithm makes the error negligible. Putting $\mu=k_BT_F$, where T_F is the Fermi temperature,

$$P(0)=2\pi(m_1m_2)^{1/2}\mu[1-\tfrac{1}{2}(m_+^*/m_3)(T/T_F)]. \tag{A7}$$

ii. $K_z=k_F$. We define the Fermi momentum along the Z axis by

$$k_F^2/2m_3=\mu. \tag{A8}$$

---

[10] W. Harrison, Phys. Rev. **131**, 2433 (1963).

By an obvious transformation, we write (A4) as

$$P(k_F)=\left(\frac{4\pi k_BTm_1m_2m_3}{m_+{}^*}\right)^{1/2}\int_{-\infty}^{\infty}dx\exp\left(-\frac{m_3x^2}{m_+{}^*k_BT}\right)\ln\left\{1+\exp\left[-\frac{1}{k_BT}(x^2+2x\mu^{1/2})\right]\right\}. \tag{A9}$$

When x is positive, the logarithmic term and the Gaussian both go to zero very fast, and we shall only need an asymptotic evaluation of that part. For negative x, the logarithmic term has a maximum at $|x|\sim\mu^{1/2}$ and we can evaluate it as above.

$$I_-=\left(\frac{4\pi k_BTm_1m_2m_3}{m_+{}^*}\right)^{1/2}\int_{-\infty}^{0}\exp\left(-\frac{m_3x^2}{m_+{}^*k_BT}\right)\ln\left\{1+\exp\left[-\frac{1}{k_BT}(x^2+2x\mu^{1/2})\right]\right\}dx$$

$$\simeq(4\pi m_1m_2k_BT\mu)^{1/2}\left(\frac{m_+{}^*}{m_3}\right)^{1/2}-\frac{\pi}{2}k_BT(m_1m_2)^{1/2}\frac{m_+{}^*}{m_3}. \tag{A10}$$

For positive x, we have

$$I_+=\left(\frac{4\pi k_BTm_1m_2m_3}{m_+{}^*}\right)^{1/2}\int_{0}^{\infty}\exp\left(-\frac{m_3x^2}{m_+{}^*k_BT}\right)\ln\left\{1+\exp\left[-\frac{1}{k_BT}(x^2+2x\mu^{1/2})\right]\right\}dx. \tag{A11}$$

For low temperatures, we can make an expansion:

$$\ln\left\{1+\exp\left[-\frac{1}{k_BT}(x^2+2x\mu^{1/2})\right]\right\}=\sum_{n=1}^{\infty}(-)^{n-1}\frac{\exp\left[-\frac{n}{k_BT}(x^2+2x\mu^{1/2})\right]}{n}. \tag{A12}$$

Now

$$I_n=\int_0^{\infty}dx\exp\left[-\frac{m_3x^2}{m_+{}^*k_BT}-\frac{n}{k_BT}(x^2+2x\mu^{1/2})\right]$$

$$=\left(\frac{m_+{}^*k_BT}{m_3+nm_+{}^*}\right)^{1/2}\exp\left[\frac{n^2\mu m_+{}^*}{k_BT(m_3+nm_+{}^*)}\right]\mathrm{Erfc}\left(\frac{n(\mu m_+{}^*)^{1/2}}{[k_BT(m_3+nm_+{}^*)]^{1/2}}\right). \tag{A13}$$

Taking the error function,[11]

$$\mathrm{Erfc}(x)=\int_x^{\infty}e^{-t^2}dt=\tfrac{1}{2}x^{-\frac{1}{2}}e^{-\frac{1}{2}x^2}W_{-\frac{1}{4},\frac{1}{4}}(x^2) \tag{A14}$$

$$\simeq\tfrac{1}{2}(e^{-x^2}/x).$$

$W_{k,m}(Z)$ is the Whittaker function, and the last line is obtained by using the known asymptotic formula for $W_{k,m}(Z)$.[11] So for small T,

$$I_n=(1/2n)\cdot(k_BT/\mu^{1/2}), \tag{A15}$$

and

$$\sum_{n=1}^{\infty}(-)^{n-1}\frac{I_n}{n}=\frac{k_BT}{2\mu^{1/2}}\sum_{n=1}^{\infty}\frac{(-)^{n-1}}{n^2}=\frac{k_BT}{2\mu^{1/2}}\tfrac{1}{2}\cdot\zeta(2) \tag{A16}$$

$$=\pi^2k_BT/24\mu^{1/2}.$$

$\zeta(Z)$ is the Reimann Zeta function of argument Z.[11] Thus

$$I_+=\left(\frac{4\pi k_BTm_1m_2m_3}{m_+{}^*}\right)^{1/2}\frac{\pi^2k_BT}{24\mu^{1/2}}. \tag{A17}$$

Collecting (A10) and (A17), we get

$$P(k_F)=(4\pi m_1m_2k_BT\mu)^{1/2}\left(\frac{m_+{}^*}{m_3}\right)^{1/2}-\frac{\pi}{2}k_BT(m_1m_2)^{1/2}\frac{m_+{}^*}{m_3}+\left(\frac{4\pi k_BTm_1m_2m_3}{m_+{}^*}\right)^{1/2}\frac{\pi^2k_BT}{24\mu^{1/2}}. \tag{A18}$$

---

[11] E. T. Whittaker and G. N. Watson, *Modern Analysis* (Cambridge University Press, New York, 1958).

We now calculate the ratio

$$\frac{P(k_F)}{P(0)}=\frac{1}{\pi^{1/2}}\left(\frac{m_+^*T}{m_3T_F}\right)^{1/2}-\frac{1}{4}\frac{m_+^*T}{m_3T_F}+\frac{1}{2\pi^{1/2}}\left(\frac{m_+^*T}{m_3T_F}\right)^{3/2}+\frac{\pi^{3/2}}{24}\left(\frac{m_3}{m_+^*}\right)^{1/2}\left(\frac{T}{T_F}\right)^{3/2}. \tag{2.4}$$

To get the result for the spherical energy surface, we have to put $m_1=m_2=m_3=m$.

APPENDIX B

In this Appendix we calculate the momentum distribution of electrons in the presence of static impurities. A detailed discussion of this problem is found in the papers of S. F. Edwards and J. S. Langer.[12] We shall give a short summary of the calculation.

We consider a gas of independent electrons inside which there is a small concentration of randomly distributed impurities, assumed fixed in their positions. The Hamiltonian of the system is

$$H=\sum_{\mathbf{k}}\tilde{\epsilon}_{\mathbf{k}}b_{\mathbf{k}}^{\dagger}b_{\mathbf{k}}+\sum_{\mathbf{k},\mathbf{q},q\neq 0}v(\mathbf{q})\rho(\mathbf{q})b_{\mathbf{k+q}}^{\dagger}b_{\mathbf{k}}. \tag{B1}$$

Here

$$\tilde{\epsilon}_{\mathbf{k}}=\epsilon_{\mathbf{k}}-\mu,$$

$$v(\mathbf{q})=(1/\Omega)\int e^{-i\mathbf{q}\cdot\mathbf{x}}v(\mathbf{x})d\mathbf{x}, \tag{B2}$$

$v(\mathbf{x}-\mathbf{R}_s)$ being the potential due to scattering center at $\mathbf{R}_s$ and supposed to be central, so that $v(\mathbf{q})$ depends on the magnitude of $\mathbf{q}$ only. $\rho(\mathbf{q})$ is defined by

$$\rho(\mathbf{q})=\sum_s e^{-i\mathbf{q}\cdot\mathbf{R}_s}, \tag{B3}$$

where the sum is performed over all the impurity positions $\mathbf{R}_s$ in some configuration. We shall average over different configurations later. In (B1), we have neglected effects of spin of electrons or impurities altogether, an assumption evidently valid for impurities without strong magnetic interaction.

The problem now is to calculate the single-particle Green's function of the electrons. For a particular configuration of impurities, the system is not homogeneous and the Green's function will not be diagonal in momentum space. We therefore start by considering the Green's function of the form[13]

$$G(\mathbf{k},\mathbf{k}';t-t')=(-i)\langle T(b_{\mathbf{k}}(t)b_{\mathbf{k}'}^{\dagger}(t'))\rangle. \tag{B4}$$

One can similarly define a retarded and an advanced Green's function:

$$\begin{aligned}G_r(\mathbf{k},\mathbf{k}';t-t')&=(-i)\theta(t-t')\langle\{b_{\mathbf{k}}(t),b_{\mathbf{k}'}^{\dagger}(t')\}\rangle,\\ G_a(\mathbf{k},\mathbf{k}';t-t')&=i\theta(t-t')\langle\{b_{\mathbf{k}}(t),b_{\mathbf{k}'}^{\dagger}(t')\}\rangle.\end{aligned} \tag{B5}$$

All three of them satisfy the same equation of motion:

$$\left(i\frac{\partial}{\partial t}-\tilde{\epsilon}_{\mathbf{p}}\right)G(\mathbf{p},\mathbf{p}';t-t')=\delta(t-t')\delta_{\mathbf{p},\mathbf{p}'}+\sum_{\mathbf{q}}v(\mathbf{q})\rho(\mathbf{q})G(\mathbf{p}-\mathbf{q},\mathbf{p}';t-t'). \tag{B6}$$

Take the Fourier transform

$$G(\mathbf{p},\mathbf{p}';t-t')=\frac{1}{2\pi}\int_{-\infty}^{\infty}G(\mathbf{p},\mathbf{p}';\omega)e^{-i\omega(t-t')}, \tag{B7}$$

and define

$$G^{\circ}(\mathbf{p},\omega)=1/(\omega-\tilde{\epsilon}_{\mathbf{p}}). \tag{B8}$$

Hence (B6) gives

$$G(\mathbf{p},\mathbf{p}';\omega)=G^{\circ}(\mathbf{p},\omega)\delta_{\mathbf{p},\mathbf{p}'}+G^{\circ}(\mathbf{p},\omega)\sum_{\mathbf{q}}v(\mathbf{q})\rho(\mathbf{q})G(\mathbf{p}-\mathbf{q},\mathbf{p}';\omega). \tag{B9}$$

Following Edwards,[12] we try to obtain a simple perturbation solution for (B9) when the concentration of impurities is low. By iteration,

$$\begin{aligned}G(\mathbf{p},\mathbf{p}';\omega)={}&G^{\circ}(\mathbf{p},\omega)\delta_{\mathbf{p},\mathbf{p}'}+G^{\circ}(\mathbf{p},\omega)\sum_{\mathbf{q}}v(\mathbf{q})\rho(\mathbf{q})G^{\circ}(\mathbf{p}-\mathbf{q};\omega)\delta_{\mathbf{p}-\mathbf{q},\mathbf{p}'}\\ &+G^{\circ}(\mathbf{p},\omega)\sum_{\mathbf{q}_1}v(\mathbf{q}_1)\rho(\mathbf{q}_1)G^{\circ}(\mathbf{p}-\mathbf{q}_1,\omega)\sum_{\mathbf{q}_2}v(\mathbf{q}_2)\rho(\mathbf{q}_2)G^{\circ}(\mathbf{p}-\mathbf{q}_1-\mathbf{q}_2;\omega)\delta_{\mathbf{p}-\mathbf{q}_1-\mathbf{q}_2,p'}+\cdots.\end{aligned} \tag{B10}$$

We shall now average over the configuration of the impurities. The averaging process was discussed in detail by Kohn and Luttinger[14] and is explained in the article of Edwards. This restores momentum conservation in the

---

[12] S. F. Edwards, Phil. Mag. **3**, 1020 (1958); J. S. Langer, Phys. Rev. **120**, 714 (1960).

[13] D. N. Zubarev, Usp. Fiz. Nauk **71**, 71 (1960) [English transl.: Soviet Phys.—Usp. **3**, 320 (1960)].

[14] W. Kohn and J. M. Luttinger, Phys. Rev. **108**, 590 (1957).

propagator as the medium becomes homogeneous. We have

$$\begin{aligned} \langle G(\mathbf{p},\mathbf{p}';\omega)\rangle &= \bar{G}(\mathbf{p},\omega)\delta_{\mathbf{p},\mathbf{p}'}\,, \\ \langle \rho(\mathbf{q})\rangle &= 0\,, \\ \langle \rho(\mathbf{q}_1)\rho(\mathbf{q}_2)\rangle &= N_i\delta(\mathbf{q}_1+\mathbf{q}_2)\,, \\ \langle \rho(\mathbf{q}_1)\rho(\mathbf{q}_2)\rho(\mathbf{q}_3)\rangle &= N_i\delta(\mathbf{q}_1+\mathbf{q}_2+\mathbf{q}_3)\,, \\ \langle \rho(\mathbf{q}_1)\rho(\mathbf{q}_2)\rho(\mathbf{q}_3)\rho(\mathbf{q}_4)\rangle &= N_i\delta(\mathbf{q}_1+\mathbf{q}_2+\mathbf{q}_3+\mathbf{q}_4)+N_i^2\sum{}^{(2)}\,\delta(\mathbf{q}_1+\mathbf{q}_2)\delta(\mathbf{q}_3+\mathbf{q}_4)\,, \end{aligned} \tag{B11}$$

and so on. $\Sigma^{(2)}$ implies a sum over similar sets of two δ functions obtained by selecting two momenta out of the four. N_i is the total number of impurities present per unit volume. The first two equations in (B11) simply state that the average effect of random scatterers is zero. The third when substituted in (B10) gives the effects of the scattering on the impurities, added up one by one. The fourth and higher equations of (B11) contain the effects of multiple scattering on a single impurity, successive scattering on different impurity centers, and other complicated processes. When the concentration is low and the probability of overlap of the spheres of influence of the impurity centers small, we can simply consider the sequence of scatterings on different impurities and neglect the other terms:

$$\begin{aligned} \bar{G}(\mathbf{p},\omega) &= G^\circ(\mathbf{p},\omega)+G^\circ(\mathbf{p},\omega)[N_i\sum_{\mathbf{q}}|v(\mathbf{q})|^2G^\circ(\mathbf{p}-\mathbf{q},\,\omega)]G^\circ(\mathbf{p},\omega) \\ &\quad +G^\circ(\mathbf{p},\omega)(N_i\sum_{\mathbf{q}_1}|v(\mathbf{q}_1)|^2G^\circ(\mathbf{p}-\mathbf{q}_1,\,\omega))G^\circ(\mathbf{p},\omega)(N_i\sum_{\mathbf{q}_2}|v(\mathbf{q}_2)|^2G^\circ(\mathbf{p}-\mathbf{q}_2,\,\omega))G^\circ(\mathbf{p},\omega)+\cdots \\ &= \frac{1}{G^{\circ-1}(\mathbf{p},\omega)-\Sigma(p,\omega)} = \frac{1}{\omega-\tilde{\epsilon}_{\mathrm{p}}-\Sigma(\mathbf{p},\omega)}\,, \end{aligned} \tag{B12}$$

where

$$\begin{aligned} \Sigma(\mathbf{p},\omega) &= N_i\sum_{\mathbf{q}}|v(\mathbf{q})|^2G^\circ(\mathbf{p}-\mathbf{q};\,\omega) \\ &= N_i\sum_{\mathbf{q}}|v(\mathbf{p}-\mathbf{q})|^2G^\circ(\mathbf{q};\,\omega)\,. \end{aligned} \tag{B13}$$

In the low-concentration limit, the entire effect is thus proportional to the number of impurities present. Let us decompose Σ into real and imaginary parts:

$$\Sigma(\mathbf{p},\,\omega\pm i\epsilon)=\Delta(\mathbf{p},\omega)\mp i\Gamma(\mathbf{p},\omega)\,, \tag{B14}$$

$$\Delta(\mathbf{p},\omega)=N_i\sum_{\mathbf{q}}|v(\mathbf{p}-\mathbf{q})|^2P/(\omega-\tilde{\epsilon}_{\mathbf{q}})\,, \tag{B15}$$

$$\Gamma(\mathbf{p},\omega)=[\Omega N_i\pi/(2\pi)^3]\times\int|v(\mathbf{p}-\mathbf{q})|^2\delta(\omega-\tilde{\epsilon}_{\mathbf{q}})d\mathbf{q}\,. \tag{B16}$$

$\Gamma(p,\omega)$ represents the scattering probability of an electron from the impurities in the first Born approximation. Actually one can sum up all the multiple scatterings from the same impurity and consider a T matrix replacing the potential in (B16), so that Γ represents the true total scattering probability of an electron from the impurities. $\Delta(p,\omega)$ simply shifts the unperturbed energies and can be absorbed in the electronic effective mass.

The spectral function can now be written down from (B12). By definition, it is

$$-iA(\mathbf{p},\omega)=\lim_{\epsilon\to0}\,[\bar{G}(\mathbf{p},\,\omega+i\epsilon)-\bar{G}(\mathbf{p},\,\omega-i\epsilon)]\,, \tag{B17}$$

with ω real; and so

$$A(\mathbf{p},\omega)=2\Gamma(\mathbf{p},\omega)/[(\omega-\epsilon_{\mathrm{p}}+\mu)^2+\Gamma^2(\mathbf{p},\omega)]\,, \tag{B18}$$

where we have absorbed Δ in the effective mass.

The momentum distribution is then given by[15]

$$\begin{aligned} n_{\mathrm{p}} &= \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{A(\mathbf{p},\omega)}{e^{\beta\omega}+1} \\ &= \frac{1}{\pi}\int_{-\infty}^{\infty}d\omega\frac{1}{e^{\beta\omega}+1}\cdot\frac{\Gamma(\mathbf{p},\omega)}{(\omega-\epsilon_{\mathrm{p}}+\mu)^2+\Gamma^2(\mathbf{p},\omega)}\,. \end{aligned} \tag{3.1}$$

---

[15] P. C. Martin and J. Schwinger, Phys. Rev. **115**, 1342 (1959).