Semiclassical approach to quantum-electromagnetic excitations in metals. II

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The quantum-electromagnetic absorption in metals as a function of the external magnetic field is calculated. The theory, whose fundamental aspects were stated in a previous paper, is carried out at finite temperature. A numerical fit to the experimental results found in bismuth is made with a single free parameter. Finally the role of this parameter is discussed.

I. INTRODUCTION

Recently, following a semiclassical approach, some of the authors¹ were able to state the basic equations for the absorption and the dispersion of an electromagnetic wave propagating in metals under quantum conditions. These are the following: $\Omega \gg \omega, \, \omega \tau \gg 1, \, \epsilon_F \gg k_B T$, where Ω is the cyclotron frequency, ω the electromagnetic wave frequency, τ the relaxation time, ϵ_F the Fermi energy, k_B the Boltzmann constant, and T the absolute temperature. The existence of a quantumelectromagnetic excitation was experimentally pointed out by noting an oscillating behavior [quantum-electromagnetic oscillations (QEO)] of the microwave absorption in bismuth. The periods $\Delta(1/H)$ (where H is the external magnetic field intensity) of the oscillations were related to the cross-sectional areas of the Fermi surface.² The theory of Ref. 1 correctly took into account the existence (in the presence of an external magnetic field \vec{H}) of many values of the wave vector \vec{k} , each one related to a particular Landau level below the Fermi level, and explained a set of experimental results previously found in bismuth.² However, not all the experimental results were explained. In this paper we present an improvement of the theory which allows us to take into account more explicitly the presence of many k values, and moreover to consider more accurately the resonance linewidth in the numerical calculation of the microwave absorption. In particular, since the surface impedance derivative of the metal was also measured, the numerical fit is carried on calculating the absorption coefficient derivative $d\Gamma/dH$ as a function of H.

II. BASIC EQUATIONS

Let us shortly summarize here the general aspects of the theory developed in the previous paper.¹ In order to calculate the conductivity, the Boltzmann equation in the presence of both a static magnetic field H and the electromagnetic (em) wave was used. The equation, linearized in the wave field, was solved in the relaxation-time approximation. For the em field the time and space dependence $E \sim \exp[i(\vec{k} \cdot \vec{r} - \omega t)]$ was assumed. In the high-frequency limit, $\omega \tau \gg 1$, and high external magnetic field, $\hbar\Omega \gg (k_B T, \hbar\omega)$, each diagonal term of the conductivity tensor could be split in two parts. The first one (quantum part) gave the absorption contribution of the electrons that did not change the Landau level ($\Delta n = 0$). For these electrons the interaction with the em field was considered as a quasiparticle electron-photon interaction with energy and momentum conservation. The second diagonal term gave the classical contribution of the electrons. The nondiagonal terms of the conductivity tensor gave the Hall part. The quantum conditions were taken into account in a semiclassical way by replacing the integral $\int_0^\infty d\epsilon$ with the sum $\hbar\Omega \sum_{n}$, where *n* is the Landau quantum number. In the following, the condition $\Delta n = 0$ corresponding to $\hbar \Omega >> \hbar \omega$ is considered in the quantum term. As a conclusion, in the conductivity tensor terms of the following type appear:

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$$\Gamma_{q} = \frac{kH}{\cos\theta} \frac{f^{2}(\theta)}{\bar{\alpha}_{z}} \frac{e^{3}m_{0}^{3}}{16c\pi k_{B}T} \sum_{i}^{\infty} (n + \frac{1}{2})^{2} \cosh^{-2} \frac{\epsilon_{F} - (n + \frac{1}{2})\hbar\Omega - \frac{1}{2m_{z}} \left[\frac{\omega}{\gamma_{z}}\right]_{i}^{2}}{k_{B}T}, \qquad (1)$$

$$\Gamma_{0} = \frac{2e}{(2\pi\hbar)} \frac{m_{0}m_{c}c}{H} V(\epsilon_{F}) , \qquad (2)$$

$$\Gamma_{1} = -i\frac{\omega}{H^{2}} \frac{m_{0}^{3}c^{2}N}{\pi\bar{\alpha}_{*}\bar{\alpha}_{*}} , \qquad (3)$$

where Γ_0 gives the Hall contribution and Γ_q is the quantum term. The remaining quantities are defined in the previous paper¹ and recalled in the Appendix. In Γ_a the *n* sum runs over the Landau levels while the *i* sum runs over the possible values of ω/k ; i.e., it depends on the em dispersion law $\omega = \omega(k)$. From a physical point of view this is a consequence of the fact that, a priori, many values of the electron momentum p_z along H satisfying the conservation law exist. As we shall clarify in the following, the possible k values of the em wave which are simultaneously excited depend on the external magnetic field. This is a peculiar characteristic of the microwave absorption which distinguishes it from other types of absorption, e.g., ultrasounds. This effect allows the explanation of the experimental aspects of the QEO. Besides, the term \cosh^{-2} is present in Eq. (1) and this fact is well known in the quantum effect.³ In fact \sum_{n} in Eq. (1) gives, as a function of H, the oscillating behavior with the period $\Delta(1/H)$ directly related to the cross-sectional areas of the Fermi surface.

When the calculated values of the conductivity σ_{ik} are put in the Maxwell equations, it is possible to obtain from the consistency conditions a set of equations for the absorption and dispersion of the em field. Introducing the complex variable $\omega/(kv_a) = \alpha + i\beta$, where v_a is the Alfvén velocity of the electron-hole plasma, one obtains the following equations:

$$1 - (\alpha^{2} - \beta^{2})[1 + c_{2}G^{2}(\alpha, \beta)] + c_{1}\beta G(\alpha, \beta) = 0,$$

$$2\beta[1 + c_{2}G^{2}(\alpha, \beta)] + c_{1}G(\alpha, \beta) = 0,$$
(4)

where

$$c_{1} = \frac{a_{xx} + a_{yy}}{(b_{xx} + b_{yy})^{1/2}} \frac{(\pi/N)^{1/2}c^{3}}{4\pi c^{3}m_{0}^{3/2}k_{B}T} \times \frac{f^{2}(\theta)(\bar{\alpha}_{x}\bar{\alpha}_{y})^{1/2}}{\bar{\alpha}_{z}\cos\theta}H^{2}, \qquad (5)$$

$$c_2 = c_1^2 \frac{a_{xx} a_{yy}}{(a_{xx} + a_{yy})^2} , \qquad (6)$$

$$G(\alpha,\beta) = \sum_{n=0}^{\infty} (n + \frac{1}{2})^{2} \cosh^{-2}a (x_{n}^{2} - \alpha^{2} + \beta^{2}),$$
(7)
$$x_{n}^{2} = \frac{2\overline{\alpha}_{z} \cos^{2}\theta}{v_{a}^{2}m_{0}} \left[\epsilon_{F} - (n + \frac{1}{2}) \frac{\hbar eH}{m_{0}c} (\overline{\alpha}_{x}\overline{\alpha}_{y})^{1/2} \right],$$
(8)

where the product $c_1 G(\alpha, \beta)$ is essentially the quantum term, c_2 is proportional to the angle between the principal planes of the energy constant surfaces, and the plane of rotation of \mathbf{H} , x_n is the velocity (in units of v_a) of the electrons of the *n*th Landau level at $\epsilon = \epsilon_F$. The other quantities are given in the Appendix. We recall that in Eqs. (4) – (8) an ellipsoidal dispersion law for the carriers has been used. Introducing the variable $\xi = \alpha^2 - \beta^2$, one obtains from Eq. (4),

$$F(\xi) = 1 - \xi^{2} [1 + c_{2} G^{2}(\xi)] - \frac{c_{1}^{2} G^{2}(\xi)}{2[1 + c_{2} G^{2}(\xi)]} = 0, \qquad (9)$$

whose solutions $\overline{\xi}_i$ allow to calculate the absorption which is found to be

$$\beta(H) = -\sum_{i} \frac{c_1 G(\xi_i)}{2[1 + c_2 G^2(\overline{\xi}_i)]} , \qquad (10)$$

where \sum_{i} runs over the possible solutions of Eq. (9). The values $\overline{\xi}_i$ for which Eq. (9) is satisfied are included in the range 0-1 and are less than or equal to the number n_F of Landau levels below the Fermi level. In other words, the branches $\omega(\vec{k})$ are a priori n_F at the most. The function $F(\xi)$ strongly depends on the magnetic field H intensity. As can be seen in Fig. 1, $F(\xi)$ presents a minimum for each value of n. In this figure $F(\xi)$ is plotted for different values of H.

In the previous paper,¹ in order to calculate $\beta(H)$ we supposed that the values $\overline{\xi}_i$ were approxi-



FIG. 1. Behaviors of the function $F(\xi)$ for different values of the external magnetic field H.

mated by those for which the function $F(\xi)$ shows a relative minimum; in other words, the limit $T \rightarrow 0$ was assumed (thermal-line width equal to zero). The theoretical conclusions were only qualitatively in agreement with the experiments, while some results were not explained. In the following we shall carry out the calculation of $d\beta/dH$, taking into account the width of the thermal line in $F(\xi)=0$, and show how it is possible to fit the experimental data with one parameter only. In particular the theory will be able to explain the QEO modulations which, as we have shown in Ref. 4, cannot be related to the simultaneous presence of different charge carrier pockets in momentum space, but are a peculiar feature of the QEO.

III. SOLUTION OF $F(\xi)=0$ WITH FINITE THERMAL LINE

To clarify the problem let us consider Fig. 1, which gives the function $F(\xi)$. It consists of a set of spikes along the line $y = 1 - \xi$. The spikes, when the solutions exist, intercept the ξ axis in two points which give the values $\overline{\xi}_i$ to be introduced in Eq. (10) for $\beta(H)$.

The width of these spikes is due to two possible causes: (i) the finite value of the temperature, analytically present in the quantum part of the conductivity with the term \cosh^{-2} , and (ii) the finite value of the relaxation time τ . In a previous paper² we put both $\omega \tau \rightarrow \infty$ and $T \rightarrow 0$. Here we disregard the second condition and assume $T \neq 0$. In order to do this let us suppose that each spike is a function of ξ of the form

$$Y = \frac{A_i(H)}{\cosh^2 a \, (x_i^2 - \xi^2)} \,, \tag{11}$$

with

$$A_{i}(H) = Mx_{i}^{2} [1 + c_{2}(i + \frac{1}{2})^{4}] + \frac{c_{1}^{2}(i + \frac{1}{2})^{4}}{2[1 + c_{2}(i + \frac{1}{2})^{4}]}.$$
 (12)

The coefficient M will be considered as a free parameter in the further numerical fit.

Using the hypothesis of Eq. (11), $G(\overline{\xi}_i)$ is calculated first and then $\beta(H)$,

$$\beta(H) = -\sum_{i} \frac{(c_1/2A_i) \sum_{n} (n + \frac{1}{2})^2 \delta_{ni}}{1 + c_2 \left[\sum_{n} (n + \frac{1}{2})^2 \frac{\delta_{ni}}{A_i} \right]^2} .$$
 (13)

We remember that the *i* sum runs over the possible solutions of $F(\xi)=0$. The Kroenecker δ_{ni} , in Eq. (13), come from the following approximation. The values ξ_i are given by

$$\overline{\xi}_i = x_i^2 \pm \frac{1}{a} (\operatorname{arccosh} A_i)^{1/2} , \qquad (14)$$

and $G(\overline{\xi}_i)$ is

$$G(\overline{\xi}_i) = \sum_n (n + \frac{1}{2})^2 \times \cosh^{-2}a \left[x_n^2 - x_i^2 \pm \frac{1}{a} (\operatorname{arccosh} A_i)^{1/2} \right].$$
(15)

In the hypothesis of a complete separation between the spikes, the relation

$$x_n^2 - x_i^2 \gg \frac{1}{a} \tag{16}$$

is valid, and the term

$$\cosh\{a[x_n^2-x_i^2\pm\frac{1}{a}(\operatorname{arccosh} A_i)^{1/2}]\}$$

is always very large compared to 1 except when i = n. Assuming the validity of Eq. (16) one obtains Eq. (13).

The calculation of derivative $d\Gamma/dH$ of the absorption coefficient $\Gamma = v_a \beta(H)$ with respect to H is now straightforward and is reported in the Appendix. A numerical analysis of $d\Gamma/dH$ by varying H has been carried out for different values of the parameter M.

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At this point the role of M has to be stressed. It is present as a factor in the amplitude $A_i(H)$ of the lines in the function $F(\xi)$. It is clear that, in the calculation of $d\Gamma/dH$, only the lines which have amplitude such that $F(\xi)$ crosses the ξ axis give contribution to the absorption. So, in the numerical fit a condition must be imposed to the amplitude $A_i(H)$ which will analytically select the values n in the sum of Eq. (13). As previously stated, from a physical point of view not all the possible values of k, for a fixed em frequency ω , are simultaneously excited. Also, since $A_i(H)$ depends on H, one understands the twofold role played by the external magnetic field. Because of the vanishing of the argument of the hyperbolic cosine, H gives the occurrence of the resonances and by means of $A_i(H)$ the amplitude of them. The role of the parameter M is fundamental for the comparison of the experimental results obtained for bismuth with the numerical fit in two respects:

(i) The disappearance of oscillations with increasing H as given by the experimental results shown in Fig. 11 of Ref. (2),

(ii) the modulation of oscillations.⁴

In Fig. 2 we report the experimental behavior of the surface impedance derivative dR/dH as a function of M (for a certain value of the angle θ between \vec{H} and the normal to the sample surface) and the theoretical curves for three different values of M. The choice of M is carried out by imposing that the conditions (i) and (ii) be fulfilled. In Fig. 2 the value is M = 1.1. The same procedure is



FIG. 2. Theoretical behavior of the absorption derivative $d\Gamma/dH$ as a function of H for different values of the parameter M. The value M = 1.1 gives the best fit of the experimental results. θ is the angle between the magnetic field \vec{H} and the normal to the sample surface.

used for the measurements taken when H rotates in the trigonal-bisector plane. The theoretical curves together with the experimental ones are given in Fig. 3 for different values of θ . The values found for *M* are also reported.

IV. CONCLUSION

The improvement of the theory in the semiclassical approach, obtained by means of a careful evaluation of the linewidth of the resonance, enables one to explain a set of experimental results of the microwave absorption in bismuth. In particular the main result of this paper consists of the fact that, with only one parameter M, we can fit at the same time both the magnetic field range in which the oscillations disappear and the periods of the modulations. This is summarized in Fig. 3, where the agreement between experimental and theoretical curves is surprisingly good.

Beyond the fact that we are able to explain the experimental results, some comments on the role of the parameter M are necessary. Varying M the theoretical behavior of $d\Gamma/dH$ as a function of H presents the following characteristics:

(i) For low values of M there are no oscillations due to the fact that the function $F(\xi)$ is always different from zero.

(ii) With increasing M a large peak appears for H = 4 kG.

(iii) By further increasing M the oscillations ap-



FIG. 3. Experimental and theoretical fit for different values of the angle ϑ .

pear with a modulation superimposed on them (Fig. 3).

(iv) For high values of M the oscillations are present without modulation and do not disappear for high values of H.

To clarify more precisely the physical meaning of this parameter one has to solve the conductivity equations without the condition $\omega \tau \rightarrow \infty$. This is a very hard problem whose solution will be attempted in the future.

APPENDIX

Assuming for the carriers an ellipsoidal dispersion law centered at the origin of the momentum space with the z axis along the external magnetic field,

$$\epsilon = (a_{11}p_x + a_{22}p_y + a_{33}p_z + 2a_{12}p_xp_y + 2a_{13}p_xp_z + 2a_{23}p_yp_z)\frac{1}{2m_0},$$

the quantities defined in the paper are as follows:

$$\begin{aligned} f^{2}(\theta) &= \left[(\overline{\alpha}_{x})^{1/2} \sin\alpha \sin\theta + (\overline{\alpha}_{x})^{1/2} \cos\theta(\gamma_{x} \cos\alpha + \gamma_{y} \sin\alpha) \right]^{2} / m_{0}^{2} \\ &+ \left[(\overline{\alpha}_{y})^{1/2} \cos\alpha \sin\theta + (\overline{\alpha}_{y})^{1/2} \cos\theta(\gamma_{y} \cos\alpha - \gamma_{x} \sin\alpha) \right]^{2} / m_{0}^{2} , \\ \gamma_{z} &= \frac{\overline{\alpha}_{z}}{k_{z}m_{0}} , \\ \overline{\alpha}_{x} &= a_{11} \cos^{2}\alpha + a_{22} \sin^{2}\alpha + a_{12} \sin\alpha \cos\alpha , \\ \overline{\alpha}_{y} &= a_{11} \sin^{2}\alpha + a_{22} \cos^{2}\alpha - a_{12} \sin\alpha \cos\alpha , \\ \overline{\alpha}_{z} &= a_{33} + a_{22} \gamma_{y}^{2} + a_{12} \gamma_{x} \gamma_{y} + a_{11} \gamma_{x}^{2} - a_{13} \gamma_{x} - a_{23} \gamma_{y} , \\ a_{xx} &= \frac{\overline{\alpha}_{x} \overline{\alpha}_{y} (\sin\theta + \gamma_{y} \cos\theta)^{2}}{\alpha_{x} A'^{2} + \alpha_{y} B'^{2}} , \end{aligned}$$

$$a_{yy} = \frac{\alpha_x \gamma_x \alpha_y}{\alpha_x A'^2 + \alpha_y B'^2},$$

$$b_{xx} = \frac{\alpha_x \cos^2 \alpha + \alpha_y \sin^2 \alpha}{\alpha_x \alpha_y} + \cdots,$$

$$b_{yy} = \frac{\alpha_x (\gamma_x \cos \alpha + \gamma_y \sin \alpha)^2 + \alpha_y (\gamma_y \cos \alpha - \gamma_x \sin \alpha)^2}{\alpha_x \alpha_y} + \cdots,$$

$$\bar{\delta} = \left(\frac{2a_y - \sin^2 \theta + a_x}{\bar{\alpha}_x \bar{\alpha}_y}\right)_{\text{electrons}} + \cdots,$$

(where the ellipses represent an analogous term for holes)

$$v_a = \frac{H}{(4\pi^2 m_0 \overline{\delta} N)^{1/2}} ,$$

and α is the angle between the principal planes of the energy constant surface and the plane in which H rotates,

$$\tan \alpha = \frac{-(a_{11}-a_{22}) \pm [(a_{11}-a_{22})^2 + a_{12}^2]^{1/2}}{a_{12}},$$

.

$$\gamma_{x} = \frac{a_{22}a_{13} - a_{23}a_{12}}{a_{12}a_{22} - a_{12}^{2}} ,$$

$$\gamma_{y} = \frac{a_{11}a_{23} - a_{13}a_{12}}{a_{11}a_{22} - a_{12}^{2}} ,$$

 $A' = \sin\theta \sin\alpha + \cos\theta(\gamma_x \cos\alpha + \gamma_y \sin\alpha) ,$

 $B' = \sin\theta \cos\alpha + (\gamma_y \cos\alpha - \gamma_x \sin\alpha) ,$

$$\frac{d\Gamma}{dH} = -\left[\frac{v_a}{H}\right] \frac{(n+\frac{1}{2})^2 / A_n}{1+c_2 [(n+\frac{1}{2})^2 / A_n]^2} + \frac{(n+\frac{1}{2})^2}{A_n} \frac{\left[1-\frac{D_n}{2A_n}\right] \left[1-c_2 \left[\frac{(n+\frac{1}{2})^2}{A_n}\right]^2\right]}{\left[1+c_2 \left[\frac{(n+\frac{1}{2})^2}{A_n}\right]^2\right]^2},$$

where

$$D_n = \frac{c_1^2 (n + \frac{1}{2})^4}{\left[1 + c_2 (n + \frac{1}{2})^4\right]^2} - \left[x_n^2 \left[1 - 3c_2 (n + \frac{1}{2})^4\right] + \frac{\epsilon_F}{2k_B T a} \left[1 + c_2 (n + \frac{1}{2})^4\right]\right]$$

and

$$a = \frac{v_a^2 m_0}{4k_B T \overline{\alpha}_z \cos^2 \theta} \; .$$

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