IMPURITY STATE OF GRAPHITE IN THE QUANTUM LIMIT

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§1. Introduction

Brandt et al have carried out detailed experiments on the galvanomagnetic properties of graphite in magnetic field ranged from 200 Oe to 500 kOe. (1) They observed that in fields H > 200 kOe $|\sigma_{xy} H|$ decreases sharply with H. (see Fig.1) In strong magnetic field $\sigma_{xy} H$ is given by

$$\sigma_{xy} H = ec(p - n), \quad (e > 0), \qquad (1.1)$$

where p and n denote hole and electron concentrations, respectively. Charge neutrality needs the following condition:

$$p - n = \sum_i \left(\frac{e_i}{e}\right) z_i N_i, \qquad (1.2)$$

where z_i denotes the valence of the i-th impurity and N_i its concentration.

Brandt et al ascribed the decrease of $|\sigma_{xy} H|$ to the freeze-out of carriers. They conjectured that the similar effect predicted by YKA theory in semiconductors (2), can occur in graphite. Namely, $a_B^* < r_s$ holds, where a_B^* denotes the Bohr radius of an impurity electron and r_s is the screening radius of current carriers. In graphite the condition $a_B^* < r_s$ is not satisfied in zero magnetic field, then bound states are not formed, but intense magnetic field changes the condition necessary for occurance of magnetic freeze-out. As H increases, the effective Bohr radius a_B^* decreases and the binding energy E_B increases, accordingly the bound states, which trap current carriers, are formed.

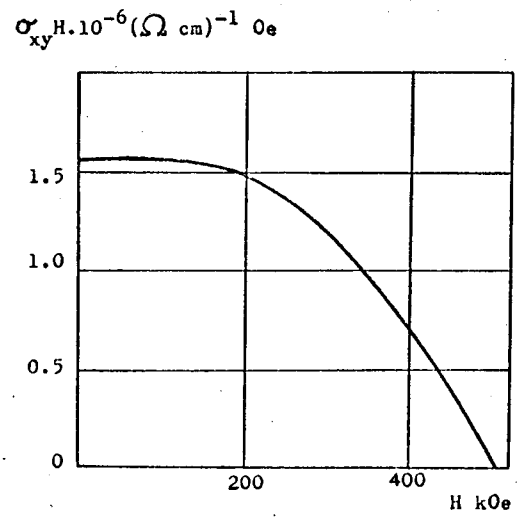

Fig.1 σ_{xy}H vs H curve in graphite (T = 4.2 K)

However, it seems to be doubtful to apply the theory of the freeze-out effect in semiconductors to semimetallic graphite. In this article we present a theory describing an impurity state in graphite in the quantum limit by extending the theories of Koster-Slater, Koster, Wolf, and Clogston. (3 ~ 6) As will be stated later, we can show that feature of the Landau states in graphite make appearance of the bound states possible for $H > H_c$, where H_c ($\cong$ 70 kOe) correspond to the quantum limit field strength.

§2. Scattering of Landau Electrons

In a field of an impurity potential V(r) an incoming state Ψ_λ is related to an outgoing scattered wave as follows:

$$\Psi = \Psi_\lambda + (\varepsilon - \mathcal{H}_0 + i\eta)^{-1} V \Psi, \qquad (2.1)$$

where λ indicates a Landau state and $\mathcal{H}_0$ is the unperturbed Hamiltonian. (7)
Let us expand Ψ by the Wannier function (3 ~ 6),

$$\Psi = N^{-1/2} \sum_{t=1}^{4} \sum_n U_t(R_n) w_t(r - R_n), \qquad (2.2)$$

where t = 1 ~ 4 corresponds to the bands E_1, E_2, E_3, and E_3' (8), and N is a number of the unit cell.

By neglecting γ_3 the Landau state Ψ_λ is given by

$$\Psi_\lambda = \sum_{t=1}^{4} c(\lambda_t) u_{N_t}(x - X) e^{ik_y y} \phi_{k_z}^{(t)}, \qquad (2.3)$$

where

$$X = \frac{k_y}{s}, \quad s = \frac{eH}{\hbar c},$$

and $\phi_{k_z}^{(t)}$ is the Bloch function at $k_x = k_y = 0$.

By expanding $V\Psi$ into the Landau states and operating

$$\int d\tau\, \overline{w_t(r - R_n)} \ldots,$$

we get

$$U_t(R_o) \cong A(\lambda_t) + N^{-1}\sum_{\mu}|c(\mu_t)|^2(\varepsilon-\varepsilon_\mu+i\eta)^{-1} \times \sum_s V_{ts}U_s(R_o) , \qquad (2.4)$$

where

$$\begin{cases} A(\lambda_t) = c(\lambda_t)u_{N_t}(X_o-x)e^{ik_yY_o}e^{-ik_zZ_o}, \\ \int d\tau\, \overline{w_s(r-R_m)}V(r)w_{s'}(r-R_n) \cong V_{ss'}\,\delta_{mn}. \end{cases}$$

In deriving (2.4) we assumed that $V(r)$ is well localized around $R_o(X_o, Y_o, Z_o)$. Due to the presence of $C(\mu_t)$ it is difficult to solve the simultaneous equation (2.4). To obtain the condition of the bound state formation is eqivalent to find in what situation $U_t(R_o)$ becomes infinite.

§3. Bound state in graphite

It is more easier to treat $U(R_o) = \sum_t U_t(R_o)$ instead of $U_t(R_o)$. For simplicity we put

$$\sum_s V_{ts}U_s(R_o) = V_o \sum_s U_s(R_o) = V_oU(R_o), \qquad (3.1)$$

and assume V_o as a constant. Thus, we get

$$U(R_o) = \frac{A_\lambda}{D(\varepsilon)}, \quad A_\lambda = \sum_t A(\lambda_t). \qquad (3.2)$$

Introducing a quantity

$$\varphi = \frac{1}{2}c_ok_z, \quad c_o\text{: unit cell height}, \qquad (3.3)$$

$D(\varepsilon)$ is represented by

$$D(\varepsilon) = 1 - V_o\left\{\sum_\mu \frac{\Omega s}{2\pi^2c_o}\int d\varphi\, P\left(\frac{1}{\varepsilon-\varepsilon_\mu(\varphi)}\right) - i\pi\Omega\sum_\mu g_\mu(\varepsilon)\right\}, \qquad (3.4)$$

$g_\mu(\varepsilon)$: density of state related to μ-th level, Ω: unit cell volume.

The condition of the bound state formation is given by

$$\mathrm{Re}D(\varepsilon) = 0, \quad g(\varepsilon) = \sum_\mu g_\mu(\varepsilon) = 0. \qquad (3.5)$$

Carriers enter into the quantum limit at H = 70 kOe. (9,10) Landau levels at H = 70 kOe is shown in Fig.2, which indicates that any energy ε does not satisfy $g(\varepsilon) = 0$. Since $\varepsilon_o^{-1}(1) = E_3$ is a level which is independent of H, with increasing H $\varepsilon_1^{-1}(1)$ goes down, and we can find ε satisfying $g(\varepsilon) = 0$ between $\varepsilon_o^{-1}(1)$ and $\varepsilon_1^{-1}(1)$.

In strong magnetic field the quantity $a = |\mathrm{Re}D(\varepsilon) - 1|$ decreases with H. Then, if

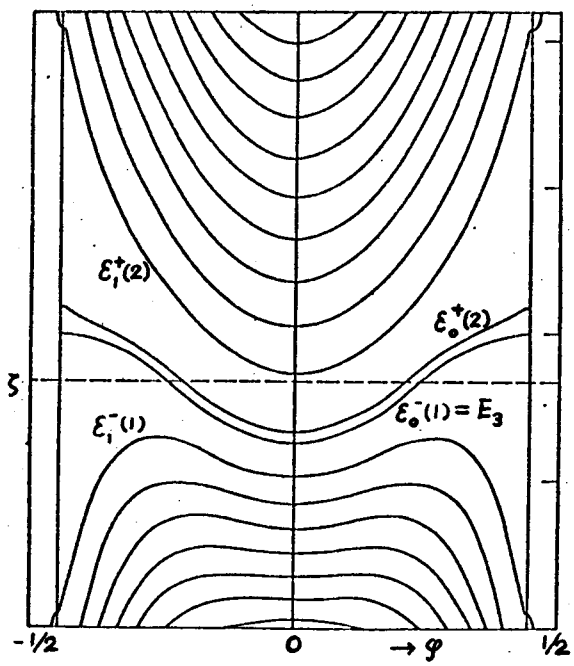

Fig.2 Landau levels for H = 70 kOe.

a is larger than unity for H < 200 kOe, the condition of $\mathrm{Re}D(\varepsilon) = 0$ can be realized with further increase of H. The consideration stated above provide a possibility of decrease of $|\sigma_{xy}H|$ in strong magnetic field.

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