ON A SPECIAL EFFECT OF $\gamma 3$ ON THE ELECTRONIC EQUIENERGY SURFACES OF GRAPHITE

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Within the framework of SLONCZEWSKI-WEISS one-electron theory of graphite the secular equation reads [1].

$$F(\kappa,\alpha) \equiv A\kappa^4 + B \cos 3\alpha\, \kappa^3 + C\,\kappa^2 + D = 0 \quad (1)$$

where κ, α are the polar radius and angle measured from the zone edge and A,B,C,D, are polynomials versus the energy ε (of degree 4,2,1 and 0 respectively) with coefficients depending on $k_z (= 2\,\Phi/Co)$.

(1) may be transformed into :

$$F(\kappa,\kappa_x) \equiv A\,\kappa^4 + (C-3B\,\kappa_x)\kappa^2 + (D+4B\,\kappa^3{}_x) = 0 \quad (2)$$

(2) is an implicite equation of κ versus κ_x which is solved in a straight-forward way. For fixed values of k_z and ε it represents the *exact form* of the k_z-cross-section of the ε-equienergy surface and we can study the effect of $\gamma 3$ on the actual form of this surface. Numerical calculus has been performed for the following parameter set :

$\gamma 0 = 3$ eV $\quad \gamma 1 = 0.3$ eV $\quad \gamma 2 = -0.018$ eV
$\gamma 4 = 0.2$ eV $\quad \gamma 5 = 0$ eV $\quad \Delta = 0.02$ eV

Figs.1 and 2 show the two general shapes of interest obtained for $\gamma 3 = 0.3$ eV and for values of ε of the same order or magnitude as the usually adopted Fermi level.

The major feature is the possibility of *a change of topology* consisting in the connection of the three off-edge "legs" of the two hole-pockets, besides the mere change of form ("trigonal warping") of the equienergy surfaces, we may also notice the consecutive disappearance of the electron-off-edge "legs" and the reduced dimensions of the electron pocket compared with those of the hole one(s).

Many consequences arise from this $\gamma 3$-effect. We particularly remark that an anomaly in the electronic density of states is expected from the *change* of topology and that the topology of Fig.2 enables the presence of *open hole-orbits*. Also, in the evaluation of the parameter set from experimental results one must eventually take account for the new topology. However no *immediate* conclusion can be drawn for the behaviour of the carriers under an applied magnetic field because of the interconnection of the γ-3 - and field - effects as shown by the work of NAKAO [2].

1. SPAIN I.L., *Chem.Phys.Carbon*, 8, 1 (1973)

2. NAKAO K., *J.Phys.Soc.Japan*, 40, 761 (1976)

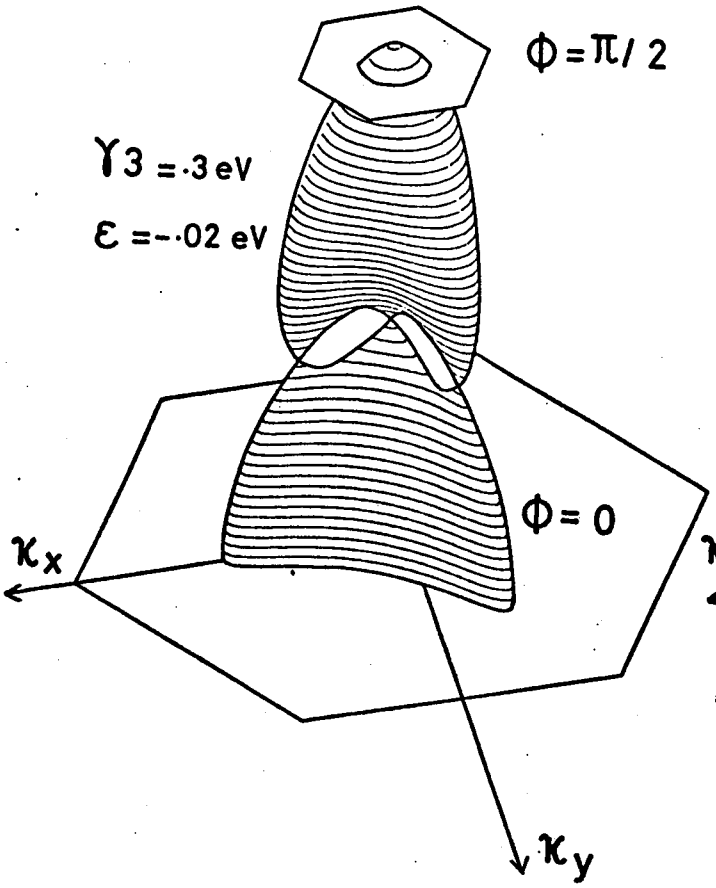

FIG.1

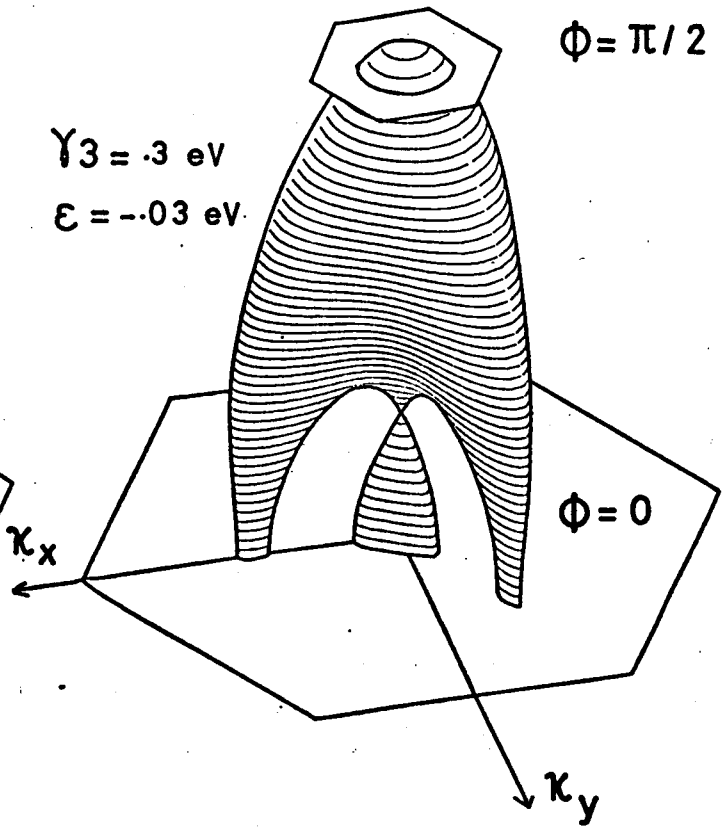

FIG. 2