## Interpretation of de Haas–van Alphen Measurements on $YBa_2Cu_3O_7$

Fowler, Freeman, Hults, King, Mueller, and Smith [1] have recently presented convincing measurements of three Fermi-surface (FS) cross sections perpendicular to the $c$ axis in $YBa_2Cu_3O_7$ using the de Haas–van Alphen effect (dHvA). The two smallest areas were assigned to the intersection of the $k_z$=0 and $k_z$=$\pi/c$ planes with a small FS cylinder (which we shall call the stick) surrounding the $S$-$R$ line $(\pi/a, \pi/b, k_z)$ at the edge of the first Brillouin zone. The larger, so-called neck area was assigned to the cross section centered at the $Z$ point $(0, 0, \pi/c)$ of the chain sheet with the $k_z$=$\pi/c$ plane. We basically agree with this assignment, but the two stick areas are substantially different and this contradicts the most recent local density approximation (LDA) calculations [2–4], which predict negligible $c$ dispersion of the corresponding band.

In this Comment we would like to point out that this apparent discrepancy can be resolved by taking into account the spin splitting of the bands due to the extremely strong applied magnetic field (100 T). We have calculated the extremal FS areas and masses in the 100 T (rigidly) spin-split band structure [5] using the same methods as in [2, 3], except that we use a substantially finer **k** mesh (845 irreducible *ab initio* points). This is necessary for an accurate description of the stick. Our results are compared with experiments in Table I. It may be seen that theory and experiment are in excellent agreement for the stick.

Our calculated extremal area for the neck is about 2.8 kT and the corresponding mass is $1.1m_e$ while the measured values are 3.51±0.10 and 7.4±2.6, respectively. Agreement between the areas may, however, be obtained by shifting the chainlike band rigidly downwards by 60 meV, which corresponds to doping with 0.05 less holes [3]. The calculated areas and masses for the 100 T spin-split bands are shown in Table I. In the experiment, the structure at 3.51 kT in the power spectral density (Fig. 2 in Ref. [1]) consists of two peaks separated by 0.17 kT. We interpret this as due to the spin splitting and the corrected experimental areas are also given in the table. As may be seen, the calculated and measured area spin splittings are in excellent agreement.

We would like to point out that the presence of a closed neck orbit is due to hybridization between the chain band and the antibonding plane band near the symmetry point $U$ $(\pi/a, 0, \pi/c)$.

TABLE I. Experimental and theoretical Fermi-surface areas and masses (LANL is the experimental values from Ref. [1]; MPI-FKF is the present LDA calculation). The $\lambda$ is the renormalization of the cyclotron mass.

| Piece | Area (kT) | Masses ($m_e$) | $\lambda$ |
|---|---|---|---|
| Stick, spin-up | | | |
| LANL | 0.53±0.02 | 7.0±2.5 | |
| MPI-FKF | 0.49 | 2.6 | 1.7±1.0 |
| Stick, spin-down | | | |
| LANL | 0.78±0.02 | 7.2±2.5 | |
| MPI-FKF | 0.75 | 3.0 | 1.4±0.8 |
| Neck, spin-up | | | |
| LANL | 3.60±0.10 | 7.4±2.6 | |
| MPI-FKF | 2.81 | 1.1 | |
| MPI-FKF[a] | 3.56 | 2.1 | 2.5±1.2 |
| Neck, spin-down | | | |
| LANL | 3.43±0.10 | 7.4±2.6 | |
| MPI-FKF | 2.71 | 1.2 | |
| MPI-FKF[a] | 3.37 | 1.7 | 3.4±1.5 |

[a]Band shifted as explained in the text.

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Received 6 February 1992
PACS numbers: 71.25.Hc, 07.55.+x, 74.60.-w

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