Comment on "Extended Van Hove Singularity in a Noncuprate Layered Superconductor Sr_2RuO_4"

In a recent Letter, Yokoya *et al.* reported the results of an angle resolved photoemission (ARPES) study of the layered perovskite superconductor Sr_2RuO_4 [1]. They interpret their spectra in terms of an extended Van Hove singularity (VHS) situated approximately 20 meV below the Fermi level and a Fermi surface (FS) consisting of two small hole sheets centered at point X of the Brillouin zone (BZ). This is in sharp contrast to the prediction of conventional energy band models [2] which yield only *one* hole surface about X and, in addition, *two* large electron sheets about Γ. It is implied in Ref. [1] that the ARPES spectra are not necessarily inconsistent, however, with other experimental measurements such as that of the de Haas–van Alphen (dHvA) and Hall effects [3,4]. In this Comment we wish to show that the converse is the case.

The dHvA measurements have revealed the existence of three distinct and essentially cylindrical FS sheets α, β, and γ which enclose volumes corresponding to 10.8%, 45.7%, and 66.7% of the Brillouin zone volume (BZV), respectively. The cyclotron masses of the quasiparticles on each sheet are also known. The electron or hole character of the sheets cannot be determined directly from a dHvA measurement in isolation, as Yokoya *et al.* [1] point out. However, if we follow the band calculations in assigning hole, electron, and electron character to α, β, and γ, respectively, we can make successful quantitative estimates of low temperature properties such as the linear heat capacity, the upper critical field, the out-of-plane conductivity, and the Hall effect [3,4].

It is important to stress that *only* this hole-electron-electron assignment for α, β, and γ is consistent with the Hall effect and Luttinger's theorem. Recent measurements [4] show that the Hall coefficient (R_H) is negative both below 30 K and above 200 K. At low temperature (<1 K) its temperature dependence is very weak, and a simple analysis based on the measured volumes of sheets α, β, and γ yields a value of R_H in agreement with the Hall effect data to an accuracy of about 20% if there are two electron sheets and one hole sheet. Any other combination inevitably yields either the wrong sign or a wildly incorrect value for R_H. Luttinger's theorem predicts that for this material, there should be an even, integral number of electrons in the BZ. Of the possible ways of assigning two electron sheets and one hole sheet to α, β, and γ, only hole-electron-electron satisfies this constraint. In fact, we can arrive at the same model of the FS even without invoking Luttinger's theorem if we note that two sheets such as β and γ that have a total volume in excess of the BZV must have the same charge character if they are to avoid crossing each other.

In contrast to the dHvA model, the ARPES FS violates Luttinger's theorem and is incompatible with measurements of the Hall effect. Neither of these deficiencies can be remedied by the addition of an unobserved electron surface mentioned in Ref. [1], unless its volume differs very considerably from that of either the β or γ surface. It is also interesting that the dHvA-measured enhancements of the quasiparticle masses over the band calculated values are similar for all three FS sheets. This suggests that the quasiparticles responsible for all the low temperature properties (including the superconductivity) are not sensitive to any sheet dependent VHS.

In conclusion, the FS model proposed by Yokoya *et al.* [1] on the basis of their ARPES spectra is in sharp, qualitative disagreement with the results of dHvA and Hall effect measurements, Luttinger's theorem, and conventional band calculations. This first detailed comparison of the results of the ARPES and the dHvA effect in a layered perovskite oxide system suggests that, contrary to the assumption often made, these methods can lead to very different results. We stress that the dHvA effect measures properties of the bulk electronic structure, whereas (as acknowledged in Ref. [1]) ARPES can be sensitive to surface effects.

Note added.—Since the original submission of our Comment, new ARPES work ([5] and the following Reply) has identified a third FS sheet, whose volume differs considerably from any of those measured by dHvA. Although this means that the ARPES FS appears to be consistent with Luttinger's theorem, it further emphasizes the striking difference between the results obtained from the two techniques. The latest ARPES FS would yield dHvA frequencies of 3.0, 8.7, and 10.8 kT, instead of the measured values of 3.05, 12.7, and 18.5 kT, each of which is accurate to 1%. We also note that a temperature dependent change in FS topology would be expected to produce dramatic changes in thermal and transport properties, which are not observed.

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