Comment on "Transport at a van Hove Singularity in Cuprate Superconductors"

In a recent Letter, Newns *et al.* [1] have proposed that the universal temperature and hole concentration (p) dependence of the thermoelectric power (TEP) observed in high-T_c cuprates [2] can be explained by standard transport theory near a van Hove singularity (VHS). They focus on the data for $YBa_2Cu_3O_{7-\delta}$, alone, where for $\delta < 0.2$ the TEP, $S(T)$, is relatively temperature independent and changes both sign and slope as δ is reduced to zero. The deduced absence of the linear temperature dependence expected for a Fermi liquid led them to model the transport properties assuming a saddle point in the quasi-2D band-structure energy surface corresponding to a VHS singularity in the density of states that sweeps through the Fermi energy with carrier doping. Both $S(T)$ and the p dependence of the room-temperature TEP, $S(290)$, were qualitatively reproduced using this model.

However, $S(T)$ for $YBa_2Cu_3O_{7-\delta}$ (123) is quite different from that for the other superconducting cuprates due to additional contributions from the CuO chains, which nearly eliminate the overall temperature dependence and give $S(T)$ a small positive slope when $\delta \rightarrow 0$. The other cuprates, which lack CuO chains (i.e., excluding 123, 247, and 124), have a common linear-T dependence [2] of the form $S = S_0 - \alpha T$ where α ($\approx 0.03\,\mu V/K^2$) is positive and roughly independent of p, and S_0 has a strong universal p dependence. Figure 1 of the Letter by Newns *et al.* shows that, even in the case of 123, when the chains are significantly oxygen deficient ($\delta \approx 0.3$) the chain contribution is eliminated and the linear-T behavior is nearly completely recovered. This is best illustrated in the case of a Ca-doped 123 compound at optimum doping, i.e., $T_c = T_{c,\max}$. Here the Ca substitution overdopes the 123 cuprate, and oxygen must be removed from the chains in order to reduce p to the optimum level. Because of the oxygen disorder the metallicity of the chains is thereby destroyed and the chain contribution to the TEP is eliminated.

In Fig. 1 we show our measurements of $S(T)$ for oxygen-deficient $Yb_{0.7}Ca_{0.3}Ba_2Cu_{2.9}Co_{0.1}O_{7-\delta}$ at optimum doping (solid curve). As for the other typical optimally doped superconducting cuprates also shown in the figure (symbols), $S(T)$ is linear with negative slope and remains positive at all temperatures. With progressive oxygen loading into the overdoped region the linear T dependence is preserved so that $S(T)$ in Fig. 1 is just displaced downwards as shown in Fig. 1 by the five additional dashed curves for progressively overdoped $Yb_{0.7}Ca_{0.3}Ba_2Cu_{2.9}Co_{0.1}O_{7-\delta}$. The final curve is for a heavily overdoped composition as can be seen by the large depression in T_c. The slope does not change sign with overdoping. In the last of these, chain filling is already flattening the curve, whereas $S(T)$ for lightly to heavily overdoped $(Bi,Pb)_2Sr_2CaCu_2O_8$ samples, for example,

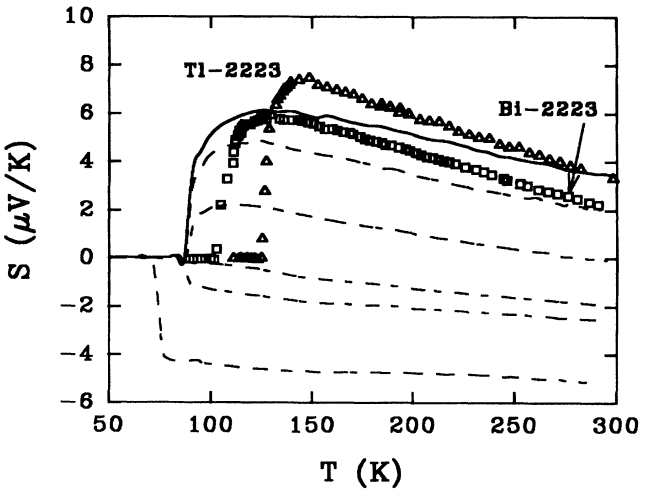

FIG. 1. The temperature dependence of the thermoelectric power $S(T)$ for optimally doped (solid curve) and progressively overdoped (dashed curves) $Yb_{0.7}Ca_{0.3}Ba_2Cu_{2.9}Co_{0.1}O_{7-\delta}$. Two other optimally doped superconducting cuprates are also shown for comparison (symbols). The linear data is displaced downwards with overdoping with no sign reversal of the slope.

keeps the same negative slope for all doping levels [3]. In short, the TEP arising from the CuO_2 planes is nowhere nearly T independent, is not symmetrical about the T axis in the underdoped and overdoped regions, and is not zero at optimum doping. For 123 the change in sign of the slope, reminiscent of that expected for a VHS but due, in fact, to contributions from nearly fully oxygenated chains [4,5], can be pushed arbitrarily far into the overdoped region by progressive Ca substitution. Finally, in the universal TEP correlation with hole concentration it is only the room temperature TEP, $S(290)$, that changes sign near (in fact beyond) optimum doping, and this cannot be relevant to the proposed VHS. There is nothing fundamental about room temperature and the more meaningful zero-temperature intercept $S_0(p)$ appears to reach zero well beyond optimum doping, at the superconductor/metal transition [2].

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Received 31 January 1995
PACS numbers: 74.25.Fy, 74.72.–h

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 0031-9007/95/75(24)/4552(1)$06.00