Comment on the paper of S. Dorbolo et al. Physica C 267 (1996) 24–30 entitled: Influence of van Hove singularity....

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In this paper, the authors analyze the influence of a saddle point (van Hove singularity) in the band structure of a 2D superconductor, on the electronic specific heat C_e and its variation with temperature. They consider only the case where the Fermi level E_F is exactly at the singularity E_s and do not study the effect of doping.

Unfortunately, their calculation is not valid because it contains several errors.

(1) To compute C_e they use the following formula:

$$C_e = \frac{d}{dT} \sum_k E_k f_k,$$

where E_k is the energy of quasiparticle excitations,

$$E_k^2 = \varepsilon_k^2 + \Delta_k^2(T).$$

This formula valid for normal metals, is in error for superconductors where E_k is T-dependent. The correct formula, given in many text books (see for example G. Rickayzen in: Superconductivity, ed. R.D. Parks, Chap. 2) the theory of Bardeen, Cooper and Schieffer (Marcel Dekker, New York, 1969, p. 79) reads

$$C_e = \sum_k E_k \, \partial f_k / \partial T.$$

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Having started from the wrong formula, all the results obtained are incorrect.

(2) The authors compute the jump in the specific heat $\Delta C / C$ at $T = T_c$ for various values of the zero temperature gap Δ_0 without changing T_c. This is also incorrect because $\Delta C / C$ is directly related to the value of the ratio $2 \Delta_0 / K_B T_c$. If one uses the correct formula for C_e, it is found that $\Delta C / C$ is directly related to the derivative $\partial \Delta^2 / \partial T$. Near T_c, one can use the formula:

$$\Delta(T) = \Delta_0 \alpha (1 - T/T_c)^{1/2}$$

(see G. Rickayzen, p. 75), where α is a numerical factor (1.74 for the simple isotropic B.C.S. model). We thus find

$$\Delta C / C \,|_{T_c} \sim (2 \Delta_0 / K_B T_c)^2.$$

In the simple B.C.S. case $2 \Delta_0 / K_B T = 3.52$ and $\Delta C / C = 1.43$.

In the case of an anisotropic gap, and in the presence of a van Hove singularity, J. Bouvier and J. Bok (Physica C 249 (1995) 117–122) have calculated the ratio $2 \Delta / K_B T_c$ and found 6.5 for the maximum gap and 2 for the minimum gap. In the case of a d-wave, Δ minimum = 0, we found $2 \Delta_0 / K_B T_c = 7.4$. In all these cases it is incorrect to change Δ_0 without changing T_c. In doing so, one may find any value whatsoever for $\Delta C / C$.

(3) There are several other errors whatsoever. Their formula (2) for the band structure $\varepsilon(k)$ is only

valid near a saddle point, at point $\overline{M}(0, \pi/a)$ for example and for an axis in k-space rotated by 45° from the (0, 1) and (1, 0) axes. But formula (4) for the d-wave gap is only valid by taking k_x along (0, 1) and k_y along (1, 0). One cannot use two different systems of axes in the same calculation. Moreover, formula (2) is incorrect far from the saddle points, so that one cannot use it for integration over the entire Fermi surface. The authors introduce three different parameters m^*, D and E_F to describe the electronic structure; in fact, there is only one independent parameter, the transfer integral t between adjacent copper atoms, the other parameters should be expressed as functions of t.

In conclusion we find that the paper by S. Dorbolo et al. contains many errors, leading to invalid conclusions.