Maximal increase of the superconducting transition temperature due to the presence of van't Hoff singularities

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In a similar way as was done previously in layered crystals {I. E. Dzyaloshinskiĭ, Pis'ma Zh. Eksp. Teor. Fiz. **46** (1987) [JETP Lett. **46** (1987)]}, the transition temperature of a bcc crystal can be increased to the critical value due to the presence of van't Hoff singularities. [*Editor's Note:* Page number for reference 1 was not provided in original Russian manuscript.] In this case $T_c \propto \exp(-\text{const}/g^{1/3})$.

In the preceding letter[1] we have examined the effect of the van't Hoff singularities on the temperature at which there is a transition in tetragonal layered crystals to which La_2CuO_4, for example, belongs. We found that the nature of the transition changes if the van't Hoff singularity occurs in the middle of the Brillouin zone surface, that there is a coherent displacement of the singlet superconductivity and of the spin-density and charge-density waves, and that the transition temperature increases[1]: $T_c \propto \exp(-\text{const}/g^{1/2})$.

Why then is the maximum increase of T_c attributable to the van't Hoff mechanism? The answer to this question lies in the straightforward generalization of the arguments advanced in Ref. 1 and in the paper by Prelovshek *et al.* cited there. Let us consider a bcc crystal and use a simple formula for the electron spectrum

$$\epsilon(\mathbf{p}) \sim \cos\frac{\pi p_1}{2p_0}\cos\frac{\pi p_2}{2p_0}\cos\frac{\pi p_3}{2p_0}. \qquad (1)$$

If there is exactly one electron per cell, the corresponding Fermi surface is a cube with the vertices (in units of p_0) A—111, B—$\bar{1}\bar{1}\bar{1}$, C—$\bar{1}11$, etc. We need now only to repeat verbatim the arguments advanced in Ref. 1.

The description of the phenomenon, as before, is determined exclusively by the neighborhoods of the points A, B, C ... . In contrast with the two-dimensional case, however, expression (1) is not a van't Hoff singularity of the general position even for a highly symmetric point at the zone boundary. In the dimensionless momenta x_1, x_2, x_3 the overall spectrum is

$$\epsilon_A = \alpha(x_1^2 + x_2^2 + x_3^2) + \beta(x_1x_2 + x_1x_3 + x_2x_3) + vp_0x_1x_2x_3 \qquad (2)$$

and the correspondingly for B, C ... . If β, $\alpha \ll vp_0$, then the overall picture of the Fermi surface, given by (1), remains the same and at temperatures T_c and chemical potentials of the transition $|\mu_c|$ (cf. Ref. 1), which lie in the interval $\alpha, \beta \ll T_c$, $|\mu_c| \ll vp_0$, the coefficients α and β in (2) may be set equal to zero.

At β, $\alpha = 0$ both the Cooper and the null-acoustic loops are cubic in the logarithms. For example,

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$$C_{AC} \sim Z_{AB} \sim \xi_1\xi_2\xi_3 \; ;$$

$$\xi_l = \ln \frac{\Lambda (v p_0)^{1/2}}{max\,(T^{1/2},\, |\mu|^{1/2},\, x_l (v p_0)^{1/2})}; \quad l = 1, 2, 3; \tag{3}$$

$\Lambda \lesssim 1$ is a dimensionless cutoff momentum. The summation of diagrams of the same order, $g\xi_1\xi_2\xi_3 \sim 1$, gives us an estimate of the transition temperature

$$T_c\,,\ |\mu_c| \sim \Lambda^2 v p_0 \exp(-\mathrm{const}/g^{1/3}), \tag{3a}$$

but it reduces, as before,[1] to the solution of equations for a fast parquet with many vertices. This problem can, however, be simplified by taking into account the periodicity of all vertices. The periods of the reciprocal (bcc) lattice are 220, ... and 400, ... Consequently, if we are considering only the neighborhood of the eight vertices of the cube in question, then 111, $1\bar{1}\bar{1}$, $\bar{1},1,\bar{1}$, and $\bar{1}\bar{1}1$ can be joined at one point A and the remaining $\bar{1}\bar{1}\bar{1}$, $\bar{1}11$, $1\bar{1}1$, and $11\bar{1}$ can be joined at the other point B. It is quite obvious that there is only one Cooper loop and one null-acoustic loop

$$C_{AB} = Z_{AB} = \frac{p_0^2}{2\pi^3 v}\, \xi_1\xi_2\xi_3 \,.$$

The corresponding parquet is described by the diagrams in Fig. 1.

The equations for a fast parquet (cf. Ref. 1) are still quite lengthy, even for a simple diagram. We will therefore restrict the discussion, as in Ref. 1, to the analysis of their polar solutions. Two vertices are mixed up in the parquet in Fig. 1: $\gamma(ABBA)$ and the vertex with the umklapp $\gamma(AABB)$. Their spin structure is given by

$$\gamma(ABBA) = \gamma_1 \delta_{\alpha\gamma}\delta_{\beta\delta} - \gamma_2 \delta_{\alpha\delta}\delta_{\beta\gamma}\,,$$
$$\gamma(AABB) = \gamma_3(\delta_{\alpha\gamma}\delta_{\beta\delta} - \delta_{\alpha\delta}\delta_{\beta\gamma}). \tag{4}$$

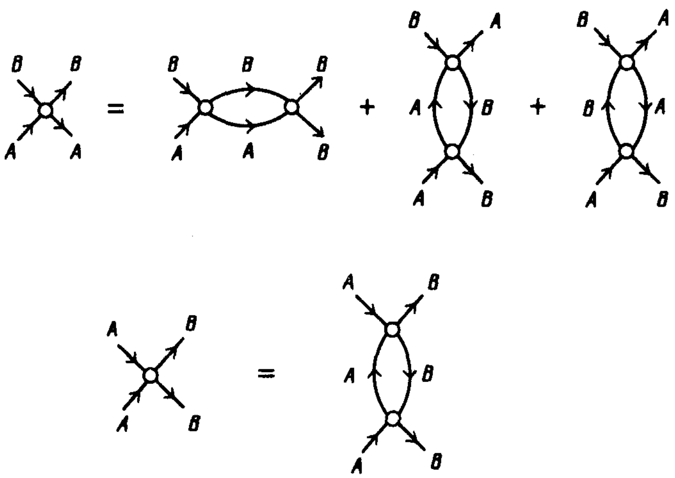

FIG. 1.

The vertices and charges are measured in units of $\pi^3 v/p_0^2$. We again have two types of poles with respect to the temperature or the chemical potential: moving and stationary. In the stationary pole ($k = 1, 2, 3$) we have

$$\gamma_k \approx \frac{\Gamma_k}{3\,\xi_0^2\,(\xi - \xi_0)}, \qquad \xi = \frac{1}{2} \ln \frac{\Lambda^2 v p_0}{max\,(T, |\mu|)}. \tag{5}$$

In the Cooper channel or the null-acoustic channel the moving poles can be written in the form

$$\gamma_k \approx \frac{\Gamma_k}{\xi\,\xi_1 \xi_2 - \xi_0^3}, \tag{6}$$

with ξ taken from (5). The position of these poles depends on the projections of the Cooper momentum **c** or the null-acoustic momentum **z**, onto the 1 and 2 axes, for example, by means of $\xi_{1,2}(\mathbf{c},\mathbf{z})$ in (6):

$$\xi_{1,2} = \ln \frac{\Lambda}{(c_{1,2}\,,\, z_{1,2})}.$$

As was explained in Ref. 1, the problem of finding and analyzing the stationary poles reduces to a single-logarithmic parquet problem, defined by the diagrams in Fig. 1, in the variables $\zeta = \xi^3$. The corresponding problem in the notation (4) was solved by Larkin *et al.*[2] The parquet is described by differential equations (9) of Ref. 2. These equations have three stationary points $(\Gamma_1 \Gamma_2 \Gamma_3)$:

$$\left(1\ \frac{1}{2}\ 0\right), \quad \left(0 - \frac{1}{2} \pm \frac{1}{2}\right).$$

All three points are stable, and the corresponding phase diagram in the space of the seed charges g_1, g_2, and g_3 is constructed in the figure in Ref. 2. At the point $(1\ \frac{1}{2}\ 0)$ the responses behave as[2]

$$\chi_{SS} \sim \chi_{CDW} \sim (1 + g_1\, \xi^3)^{-1/2}, \quad \chi_{SDW} \sim 0, \tag{7a}$$

and at the points $(0 - \frac{1}{2} \pm \frac{1}{2})$ they behave as

$$\chi_{SDW} \sim \chi_{CDW} \sim (\xi_0 - \xi)^{-1/2}, \qquad \chi_{SS} \sim 0; \tag{7b}$$

ξ_0 in (7b) is given in Ref. 2.

The Cooper channel has two poles. The (110) pole corresponds to the singlet superconductivity (SS) with a pole singularity in χ_{SS}, while the (-110) pole corresponds to the triplet pairing (TP) with the pole in χ_{TS}. The null-acoustic channel has both pure spin-density waves and pure charge-density waves with poles in χ_{SDW} and χ_{CDW}, as well as a combination of these waves.

We thus see that the triplet superconductivity is the principal feature of the cubic crystal under consideration in comparison with the tetragonal crystal considered previously.[1] Furthermore, aside from the pure states, there can also be, as before, coherent mixtures: SS + CDW and SDW + CDW.

[1]I. E. Dzyaloshinskiĭ, Pis'ma Eksp. Teor. Fiz. **46** (1987) [JETP Lett. **46** (1987)].
[2]I. E. Dzyaloshinskiĭ and A. I. Larkin, Zh. Eksp. Teor. Fiz. **61**, 791 (1971) [Sov. Phys. JETP **34**, 422 (1972)].

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