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On the Thermodynamic Critical Field for the K_3C_{60} and Rb_3C_{60} Fullerides

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In the paper the temperature dependence of the thermodynamic critical field (H_c) for the alkali-metal-doped fullerides K_3C_{60} and Rb_3C_{60} has been considered. The numerical calculations have been conducted in the framework of the Migdal-Eliashberg formalism. It has been shown that the obtained numerical values of H_c agree with the experimental data. Finally, the dimensionless ratio: $R_H \equiv T_c C^N (T_c) / H_c^2 (0)$ has been calculated, where T_c is the critical temperature and C^N denotes the specific heat in the normal state. The theoretical analysis has proved that for the considered fullerides the parameter R_H is beyond the BCS prediction. In particular: $R_H = 0.143$ for K_3C_{60}, and $R_H = 0.145$ for Rb_3C_{60}.

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For the first time the superconducting state in the alkali-metal-doped fullerides was reported in 1991 [1]. We can notice that particularly interesting were the potassium- and rubidium-doped C_{60} systems, characterized by a relatively high value of the critical temperature: $T_c = 19.5$ K (K_3C_{60}) and $T_c = 30$ K (Rb_3C_{60}) [1–5].

In the presented work the temperature dependence of the normalized thermodynamic critical field for the K_3C_{60} and Rb_3C_{60} superconductors have been studied. Due to the fact that in the considered compounds the electron-phonon interaction is strong (the electron-phonon coupling constant (λ) equals 1.22 and 1.23 for K_3C_{60} and Rb_3C_{60}, respectively [6, 7]), the calculations have been carried out in the framework of the Eliashberg formalism.

We have noticed that the appropriate Eliashberg equations have been solved by means of the iteration method, described in detail in the papers [8–13].

To calculate the thermodynamic critical field, the knowledge of the free energy difference between the superconducting and the normal state: $\Delta F \equiv F^S - F^N$ is required. The expression for ΔF has the following form [14]:

$$\frac{\Delta F}{\rho(0)} = -2\pi k_B T \sum_{n=1}^{M} \left(\sqrt{\omega_n^2 + \Delta_n^2} - |\omega_n|\right) \times \left(Z_n^S - Z_n^N \frac{|\omega_n|}{\sqrt{\omega_n^2 + \Delta_n^2}}\right), \quad (1)$$

where $\rho(0)$ denotes the electron density of states at the Fermi level, k_B represents the Boltzmann constant, and T is the temperature. The order parameter ($\Delta_n \equiv \Delta(i\omega_n)$) and the wave function renormalization factors for the superconducting and the normal state ($Z_n^S \equiv Z^S(i\omega_n)$ and $Z_n^N \equiv Z^N(i\omega_n)$) should be calculated by using the Eliashberg equations in the imaginary-axis representation ($i \equiv \sqrt{-1}$) [15]:

$$\Delta_n Z_n = \pi k_B T \sum_{m=-M}^{M} \frac{K(n,m) - \mu^\star \theta(\omega_c - |\omega_m|)}{\sqrt{\omega_m^2 + \Delta_m^2}} \Delta_m, \quad (2)$$

and

$$Z_n = 1 + \frac{\pi k_B T}{\omega_n} \sum_{m=-M}^{M} \frac{K(n,m)}{\sqrt{\omega_m^2 + \Delta_m^2}} \omega_m, \quad (3)$$

where n-th Matsubara frequency is derived from the expression: $\omega_n \equiv \pi k_B T (2n-1)$.

The electron-phonon pairing kernel is defined as:

$$K(n,m) \equiv 2 \int_0^{\Omega_{\max}} d\Omega \frac{\Omega}{(\omega_n - \omega_m)^2 + \Omega^2} \alpha^2 F(\Omega), \quad (4)$$

where the electron-phonon spectral function ($\alpha^2 F(\Omega)$) for K_3C_{60} has been obtained in [6] from the reflectance data [17]. The form of the $\alpha^2 F(\Omega)$ function for Rb_3C_{60} has been extracted from the tunnelling measurements in the paper [7]. The maximum phonon frequency $\Omega_{\max}$ is equal to 242 meV and to 100 meV for K_3C_{60} and Rb_3C_{60}, respectively.

The Coulomb pseudopotential ($\mu^\star$) describes the effects of the electron repulsion. The values of $\mu^\star$ for considered fullerides are equal to 0.39 (K_3C_{60}) and to 0.33 (Rb_3C_{60}) [7, 16]. The symbol θ denotes the Heaviside unit function and ω_c is the cut-off frequency ($\omega_c = 3\Omega_{\max}$).

The thermodynamic critical field has been calculated with the help of the expression [18] (cgs units):

$$\frac{H_c}{\sqrt{\rho(0)}} = \sqrt{-8\pi \left[\Delta F / \rho(0)\right]}. \quad (5)$$

In Figs. 1 and 2 the dependence of the normalized thermodynamic critical field on the temperature has been presented. The lines represent the theoretical calculations; the filed squares are the experimental data. It is easy to notice that the theoretical results correctly reproduce the experimental data obtained for the K_3C_{60} and Rb_3C_{60} superconductors.

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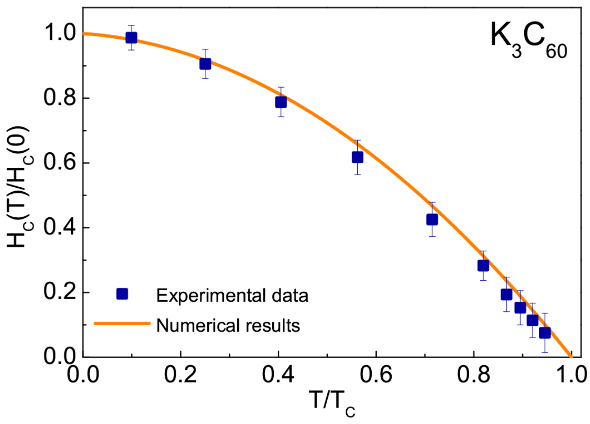

Fig. 1. The temperature dependence of the ratio $H_c(T)/H_c(0)$ for K_3C_{60} compound; $H_c(0)/\sqrt{\rho(0)}$ is equal to 16.97 meV. The experimental data have been taken from [19].

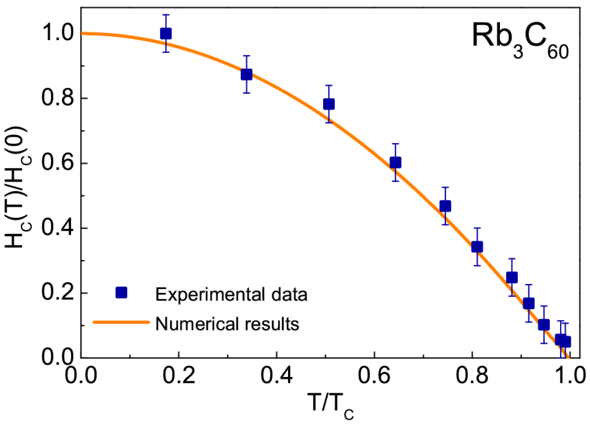

Fig. 2. The temperature dependence of the ratio $H_c(T)/H_c(0)$ for Rb_3C_{60} compound; $H_c(0)/\sqrt{\rho(0)}$ is equal to 26.03 meV. The experimental data have been taken from [20].

In the last step, the values of the dimensionless ratio: $R_H \equiv T_c C^N(T_c)/H_c^2(0)$ have been calculated, where C^N denotes the specific heat in the normal state: $C^N/\rho(0) = \gamma k_B^2 T$. The symbol γ is the Sommerfeld constant: $\gamma \equiv (2/3)\pi^2(1+\lambda)$.

In the case of the BCS theory, the parameter R_H takes the universal value of 0.168 [21]. For the K_3C_{60} and Rb_3C_{60} fullerides, we have obtained 0.143 and 0.145, respectively. We can notice that the differences between the BCS and Eliashberg results are connected with the existence of the strong-coupling and retardation effects in the K_3C_{60} and Rb_3C_{60} superconductors, which are omitted in the BCS model.

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