The Energy Gap in the $(\text{Hg}_{1-x}\text{Sn}_x)\text{Ba}_2\text{Ca}_2\text{Cu}_3\text{O}_{8+y}$ Superconductor

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Abstract The experimental data show that the increase of tin in the $(\text{Hg}_{1-x}\text{Sn}_x)\text{Ba}_2\text{Ca}_2\text{Cu}_3\text{O}_{8+y}$ superconductor results in a visible increase in the pseudogap temperature (T^*) with a slight decrease in the value of the critical temperature (T_C). Based on the above results, the dependence of the average amplitude of the energy gap on the temperature ($G(T)$) has been determined for $x \in (0, 0.25)$. On this basis, it has been found that the dimensionless ratio $R_G \equiv G(0)/k_B T_C$ increases with the increasing tin content from the value of 3.48 to the value of 4.88. Next, for $x = 0.25$ and $T \in (0, T^*)$, the dependence of the energy gap on the wave vector has been calculated in the surrounding of the Fermi level. It has been shown that in the anti-nodal region the energy gap is very weakly dependent on the temperature. On the other hand, in the nodal region its values strongly decrease together with the increasing temperature.

Keywords High- T_C superconductors · Thermodynamic properties · Electron–phonon coupling

The thermodynamic properties of the superconducting state in cuprates can be determined on the basis of two characteristic types of temperature: T_C (the critical temperature) and T^* (the pseudogap temperature). The first temperature determines the disappearance of the superconducting state; the second one represents the value below which, in the normal state, the pseudogap appears in the electron density of states [1–3].

From the physical point of view, the values of the temperatures T_C and T^* depend, among other things, on the degree of the disorder occurring between CuO_2 planes.

In the presented paper, the disorder induced by tin in the $(\text{Hg}_{1-x}\text{Sn}_x)\text{Ba}_2\text{Ca}_2\text{Cu}_3\text{O}_{8+y}$ superconductor (Sn-doped Hg-1223) has been considered. In particular, for the selected values of tin content, the dependence of the average amplitude of the energy gap on the temperature and the dependence of the energy gap on the wave vector have been calculated. The numerical analysis has been conducted in the framework of the recently introduced model [4, 5].

We notice that the model is based on the following postulates:

- (i) *In the superconductivity domain of the cuprates the fundamental role is played by the electrons on the CuO_2 planes.*
- (ii) *In the cuprates there exists the conventional electron–phonon interaction, which does not have to be strong.*
- (iii) *In the cuprates there exist strong electronic correlations, but the electron–electron scattering in the superconductivity domain is inseparably connected with absorption or emission of the vibrational quanta.*

The postulate (i) underlines the importance of the quasi two-dimensionality of the electron system. The second one draws attention to the electron–phonon pairing mechanism given by Fröhlich [6, 7]. The third one postulates that the strong electron correlations in the cuprates are coupled with the phonon degrees of freedom. The first two postulates define the van Hove scenario [8–12]. The third postulate requires further discussion because it is far more subtle. In particular, it should be noted that the postulated electron correlations generalize the Hubbard approach [13]; the classical electron–electron interaction is replaced with the electron–electron–phonon coupling.

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Fig. 1 The influence of the tin-induced disorder on the value of the temperature T_C and T^* for Sn-doped Hg-1223 [14]

Based on approach presented in the papers [4] and [5], it is possible to prove that the critical temperature uniquely determines the value of the potential for the electron–phonon interaction. On the other hand, the temperature of the pseudogap depends on both the electron–phonon potential and the potential of the electron–electron–phonon interaction. Thus, having the experimental values of T_C and T^* , it is possible to clearly determine the discussed potentials, and then calculate all relevant thermodynamic parameters of the superconducting state.

In Fig. 1, the experimental results for Sn-doped Hg-1223 obtained by Vyas and Lam are presented [14].

Looking at Fig. 1, it is easy to notice that the growth of the parameter x causes a significant increase in the pseudo-gap temperature with a weak decrease of the critical temperature value at the same time.

Based on these observations, the averaged value of the amplitude of the energy gap $G(T) \equiv 2\Delta^{(\text{tot})}(T)$ can be calculated on the basis of the following expression [4, 5]:

$$\Delta^{(\text{tot})}(T) \equiv \left(V + \frac{U}{6} |\Delta(T)|^2 \right) |\Delta(T)|, \quad (1)$$

where V and U are the attractive electron–electron pairing potentials connected with the electron–phonon and electron–electron–phonon interactions, respectively. In the first approximation, we have:

$$\frac{\omega_0 |g_{\mathbf{k}}^{(1)}(\mathbf{q})|^2}{(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}+\mathbf{q}})^2 - \omega_0^2} \rightarrow -\frac{V}{2N_0} \quad (2)$$

and

$$\frac{\omega_0 |g_{\mathbf{k},\mathbf{k}'}^{(2)}(\mathbf{q}, \mathbf{l})|^2}{(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}-\mathbf{l}} + \varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k}'+\mathbf{l}+\mathbf{q}})^2 - \omega_0^2} \rightarrow -\frac{U}{24N_0^3}, \quad (3)$$

where $N_0 \equiv 1/\sum_{\mathbf{k}}$ is the normalization constant; ω_0 represents the characteristic phonon frequency, which is of the order of the Debye frequency ($\omega_0 = 95$ meV) [15]. The symbols $g_{\mathbf{k}}^{(1)}(\mathbf{q})$ and $g_{\mathbf{k},\mathbf{k}'}^{(2)}(\mathbf{q}, \mathbf{l})$ describe the matrix elements for

Table 1 The pairing potentials V and U for Sn-doped Hg-1223 superconductor

Sn-doping	T_C (K)	T^* (K)	V (meV)	U (meV)
$x = 0.00$	134.3	206.8	7.61	36.43
$x = 0.05$	133.8	218.0	7.60	38.54
$x = 0.10$	131.7	230.5	7.53	41.25
$x = 0.15$	130.3	236.4	7.49	42.54
$x = 0.20$	127.3	251.3	7.40	45.65
$x = 0.25$	125.7	259.5	7.36	47.33

the electron–phonon and electron–electron–phonon interactions, respectively. The function $\varepsilon_{\mathbf{k}}$ denotes the band energy for the square lattice: $\varepsilon_{\mathbf{k}} = -t\gamma(\mathbf{k})$; t is the nearest-neighbor hopping integral and $\gamma(\mathbf{k}) \equiv 2[\cos(k_x) + \cos(k_y)]$. In the paper, it has been assumed that $t = 450$ meV [16].

The symbol $\Delta(T)$ in Eq. (1) denotes the averaged amplitude of the order parameter,

$$\Delta(T) \equiv \frac{1}{N_0} \sum_{\mathbf{k}} \eta(\mathbf{k}) \langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \rangle. \quad (4)$$

The function $\eta(\mathbf{k})$ has the form $\eta(\mathbf{k}) \equiv 2[\cos(k_x) - \cos(k_y)]$. The anomalous thermodynamic average is given by $\langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \rangle$; $c_{\mathbf{k}\sigma}$ is the annihilation operator of the electron state with the momentum $\mathbf{k}$ and the spin σ .

The amplitude $\Delta(T)$ should be calculated on the basis of the following equation [4]:

$$1 = \left(V + \frac{U}{6} |\Delta(T)|^2 \right) \frac{1}{N_0} \sum_{\mathbf{k}} \frac{\eta^2(\mathbf{k})}{2E_{\mathbf{k}}} \tanh \frac{\beta E_{\mathbf{k}}}{2}. \quad (5)$$

The function $E_{\mathbf{k}}$ is given by the equation

$$E_{\mathbf{k}} \equiv \sqrt{\varepsilon_{\mathbf{k}}^2 + \left(V + \frac{U}{6} |\Delta(T)|^2 \right)^2 (|\Delta(T)| \eta(\mathbf{k}))^2}, \quad (6)$$

and the quantity β has been defined by the following: $\beta \equiv 1/k_B T$ (k_B is the Boltzmann constant).

From the mathematical point of view Eq. (5) can be solved only numerically. The summation of the wave vector has been approximated with the help of the integrals,

$$\sum_{\mathbf{k}} \simeq \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} dk_x dk_y \theta(\omega_0 - |\varepsilon(\mathbf{k}_x, \mathbf{k}_y)|), \quad (7)$$

where θ denotes the Heaviside function.

The values of the pairing potentials V and U have been chosen on the basis of the temperatures T_C and T^* determined in the paper [14]. The obtained results have been presented in Table 1. It can be observed that the potential V is several times lower than the potential U . In addition,

Fig. 2 The dependence of the averaged amplitude of the energy gap on the temperature for the selected values of tin doping. The vertical red line represents the value of the critical temperature. The vertical green line represents the temperature of the pseudogap

Fig. 3 The dependence of the ratio R_G on the value of the parameter x

with the increase of tin content, the parameter V slightly decreases, whereas U significantly increases.

Taking into consideration the calculated values of V and U , with the help of Eq. (5) one can determine the dependence of the averaged amplitude of the energy gap on the temperature for the selected concentrations of tin in Hg1223 superconductor. The achieved results are presented in Fig. 2.

On the basis of the plotted courses, it is clear that in the temperature range from 0 K to T_C , the amplitude of the energy gap very weakly depends on the temperature. This result is independent of the value of the parameter x . However, with increasing tin concentration, the value of the energy gap noticeably increases.

Having the explicit form of the function $G(T)$, it is possible to determine the influence of the concentration of tin on the value of the dimensionless ratio $R_G \equiv G(0)/k_B T_C$. In the case of Sn-doped Hg-1223, the growth of the parameter x causes the increase in R_G from the value of 3.48 (this result is comparable with the result of the BCS theory [17,

18]) to the value of 4.88. The full course of the function $R_G(x)$ is presented in Fig. 3.

The results presented so far concern the properties of the energy gap, the amplitude values of which have been averaged in the vicinity of the Fermi surface. Below is the reasoning the purpose of which was to determine the dependence of the energy gap on the wave-vector with the non-averaged amplitude: $G_{\mathbf{k}}(T) \equiv 2\Delta_{\mathbf{k}}(T) = 2\eta_{\mathbf{k}}|\phi_{\mathbf{k}}|[v + u|\eta_{\mathbf{k}}||\phi_{\mathbf{k}}|^2]$, where $\phi_{\mathbf{k}} \equiv \langle c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow} \rangle$.

In the first step, the anomalous thermodynamic average has been calculated. For this purpose, the following equation has been taken into account [19]:

$$\begin{aligned} \phi_{\mathbf{k}} = & \left(\frac{1}{N_0} \sum_{\mathbf{k}_1}^{\omega_0} \eta(\mathbf{k}_1) \phi_{\mathbf{k}_1} \right) \\ & \times \left[v + u \left(\frac{1}{N_0} \sum_{\mathbf{k}_2}^{\omega_0} \eta(\mathbf{k}_2) \phi_{\mathbf{k}_2} \right) \left(\frac{1}{N_0} \sum_{\mathbf{k}_3}^{\omega_0} \eta(\mathbf{k}_3) \phi_{\mathbf{k}_3}^* \right) \right] \\ & \times \eta(\mathbf{k}) \chi_{\mathbf{k}}, \end{aligned} \quad (8)$$

where

$$\chi_{\mathbf{k}} \equiv \frac{\tan[\frac{i\beta}{2} \sqrt{\varepsilon_{\mathbf{k}}^2 + M_{\mathbf{k}}^2}]}{2i \sqrt{\varepsilon_{\mathbf{k}}^2 + M_{\mathbf{k}}^2}}. \quad (9)$$

The function $M_{\mathbf{k}}^2$ has been defined in the following way:

$$M_{\mathbf{k}}^2 \equiv \left(\frac{1}{N_0} \sum_{\mathbf{k}_1}^{\omega_0} W_{\mathbf{k}_1\mathbf{k}} \phi_{\mathbf{k}_1}^* \right) \left(\frac{1}{N_0} \sum_{\mathbf{k}_2}^{\omega_0} W_{\mathbf{k}\mathbf{k}_2} \phi_{\mathbf{k}_2} \right)$$

Fig. 4 The circles show the dependence of the energy gap on the angle for the selected values of the temperature. The red line represents the average values of the energy gap. It has been assumed that $x = 0.25$

$$\begin{aligned}
 &= \eta^2(\mathbf{k}) \left(\frac{1}{N_0} \sum_{\mathbf{k}_1}^{\omega_0} \eta_{\mathbf{k}_1} \phi_{\mathbf{k}_1}^* \right) \left(\frac{1}{N_0} \sum_{\mathbf{k}_2}^{\omega_0} \eta_{\mathbf{k}_2} \phi_{\mathbf{k}_2} \right) \\
 &\times \left[v + u \left(\frac{1}{N_0} \sum_{\mathbf{k}_3}^{\omega_0} \eta_{\mathbf{k}_3} \phi_{\mathbf{k}_3} \right) \left(\frac{1}{N_0} \sum_{\mathbf{k}_4}^{\omega_0} \eta_{\mathbf{k}_4} \phi_{\mathbf{k}_4}^* \right) \right]^2,
 \end{aligned} \quad (10)$$

where

$$W_{\mathbf{k}_1 \mathbf{k}_2} \equiv v_{\mathbf{k}_1 \mathbf{k}_2} + \frac{1}{N_0^2} \sum_{\mathbf{k}_3 \mathbf{k}_4}^{\omega_0} u_{\mathbf{k}_1 \sim \mathbf{k}_4} \phi_{\mathbf{k}_3} \phi_{\mathbf{k}_4}^*. \quad (11)$$

Additionally, $v_{\mathbf{k}_1 \mathbf{k}_2} \equiv v \eta(\mathbf{k}_1) \eta(\mathbf{k}_2)$ and $u_{\mathbf{k}_1 \sim \mathbf{k}_4} \equiv u \eta(\mathbf{k}_1) \eta(\mathbf{k}_2) \eta(\mathbf{k}_3) \eta(\mathbf{k}_4)$.

Equation (8) has been solved for 7000 points placed close to the Fermi level. The numerical procedures discussed and tested in the works have been applied (see [19–23]).

Figure 4 presents the full dependence of the energy gap on the angle α , where $\alpha \equiv \arctan(k_y/k_x)$. The calculations have been made for $x = 0.25$ and for the few selected values of the temperature.

Based on the presented results, it can be noted that in the anti-nodal region ($\alpha \sim 0$ deg) the $G(\alpha)$ values are weakly dependent on the temperature. On the other hand, the values of the energy gap from the nodal region ($\alpha \sim 45$ deg) are very low for $T > T_C$. Note that the obtained results are consistent with the results of the ARPES experiments conducted for cuprates [24, 25].

In summary, in the presented work we have determined the dependence of the energy gap averaged amplitude on the temperature for the $(\text{Hg}_{1-x}\text{Sn}_x)\text{Ba}_2\text{Ca}_2\text{Cu}_3\text{O}_{8+y}$ superconductor. The selected values of the x parameter, taken

from the range of 0 to 0.25, have been considered. It has been found that higher concentration of tin forces the dimensionless ratio R_G to increase and reach the values far beyond the value predicted by the BCS theory. In particular, $R_G \in (3.48, 4.88)$. It should be noted that this result is related to the strong growth of the electron–electron–phonon potential with an increase in the parameter x .

When conducting the studies of the superconducting properties in Sn-doped Hg-1223, the dependence of the energy gap on the angle α has been additionally determined. The rate of the concentration of tin equal to 0.25 and some selected values of the temperature have been taken into account. It has been found that in the nodal area the energy gap disappears with the increasing temperature. On the other hand, in the anti-nodal area its values are weakly dependent on the temperature. This proves the existence of the pseudogap in the electron density of states above the critical temperature.

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References

1. Bednorz, J.G., Muller, K.A.: Z. Phys. B **64**, 189 (1986)

2. Bednorz, J.G., Muller, K.A.: *Rev. Mod. Phys.* **60**, 585 (1988)
3. Dagotto, E.: *Rev. Mod. Phys.* **66**, 763 (1994)
4. Szczęśniak, R.: *PLoS ONE* **7**(4), e31873 (2012)
5. Szczęśniak, R., Durajski, A.P.: [arXiv:1206.5531](https://arxiv.org/abs/1206.5531)
6. Fröhlich, H.: *Phys. Rev.* **79**, 845 (1950)
7. Fröhlich, H.: *Proc. R. Soc. A* **223**, 296 (1954)
8. Czerwonko, J.: *J. Phys. Element. Part. At. Nucl.* **31**, 145 (2000)
9. Czerwonko, J.: *Acta Phys. Pol. B* **29**, 3885 (1998)
10. Goicochea, A.G.: *Phys. Rev. B* **49**, 6864 (1994)
11. Sarkar, S., Basu, S., Das, A.N.: *Phys. Rev. B* **52**, 12545 (1995)
12. Sarkar, S., Basu, S., Das, A.N.: *Phys. Rev. B* **51**, 12854 (1995)
13. Hubbard, J.: *Proc. R. Soc. Lond. Ser. A, Math. Phys. Sci.* **276**, 238 (1963)
14. Vyas, A., Lam, C.C.: *J. Supercond. Nov. Magn.* **14**, 487 (2001)
15. Dovhyj, Y.: *Ukr. Fiz. Zh.* **56**, 1011 (2011)
16. Pavarini, E., Dasgupta, I., Saha-Dasgupta, T., Jepsen, O., Andersen, O.K.: *Phys. Rev. Lett.* **87**, 047003 (2001)
17. Bardeen, J., Cooper, L.N., Schrieffer, J.R.: *Phys. Rev.* **106**, 162 (1957)
18. Bardeen, J., Cooper, L.N., Schrieffer, J.R.: *Phys. Rev.* **108**, 1175 (1957)
19. Szczęśniak, R., Durajski, A.P., Szczęśniak, D.: [arXiv:1302.2450v2](https://arxiv.org/abs/1302.2450v2)
20. Szczęśniak, R., Durajski, A.P., Pach, P.W.: *J. Low Temp. Phys.* **171**, 769 (2013)
21. Szczęśniak, R., Durajski, A.P.: *J. Phys. Chem. Solids* **74**, 641 (2013)
22. Szczęśniak, R., Durajski, A.P.: *Solid State Commun.* **153**, 26 (2013)
23. Szczęśniak, R., Szczęśniak, D.: *Solid State Commun.* **152**, 779 (2012)
24. Lee, W.S., Vishik, I.M., Tanaka, K., Lu, D.H., Sasagawa, T., Nagaosa, N., Devereaux, T.P., Hussain, Z., Shen, Z.-X.: *Nature* **450**, 81 (2007)
25. Damascelli, A., Hussain, Z., Shen, Z.X.: *Rev. Mod. Phys.* **75**, 473 (2003)