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Heat capacity of mesoscopically disordered superconductors: implications for MgB_2

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The electronic specific heat C as a function of temperature T is calculated for a mesoscopically disordered s-wave superconductor treated as a spatial ensemble of domains with continuously varying superconducting properties. Each domain is characterized by a certain critical temperature T_{c0} in the range $[0,T_c]$ and is supposed to have a size $L > \xi$, where ξ is the coherence length. Specific calculations are performed for exponential and Gaussian distributions of T_{c0}. For low T, the spatially averaged $\langle C(T) \rangle$ is proportional to T^2, whereas the anomaly at T_c is substantially smeared even for small dispersions. For narrow gap distributions there exists an intermediate T range, where the curve $\langle C(T) \rangle$ can be well approximated by an exponential Bardeen–Cooper–Schrieffer-like dependence with an effective gap smaller than the weak-coupling value. The results obtained successfully reproduce the salient features of the $C(T)$ data for MgB_2, where a wide superconducting gap distribution has been observed previously in the tunneling, point-contact, photoemission and Raman spectra. The conclusion is reached that the multiple-gap behavior of superconducting MgB_2 is due to the *spatial* distribution of dissimilar domains. Intrinsic nonstoichiometry of the compound or possible electronic phase separation may be the origin of the mesoscopic inhomogeneities. The same model describes the low-T heat capacity of cuprates, although the sources of inhomogeneity are different from those in MgB_2 .

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1. Introduction

After the discovery of the superconducting compound MgB_2 with a critical temperature $T_c \approx 40$ K [1] it became clear that high T_c's may be brought about not only by various exotic mechanisms such as spin-fluctuation-driven Cooper pairing [2]. Indeed, in MgB_2 the electron–phonon origin of superconductivity seems highly plausible [3–10], phonon anharmonicity probably playing a decisive role [11]. As for the symmetry of the superconducting order parameter, the available data are rather controversial, although the main body of the data correlate better with the isotropic s-wave behavior. In any case, the Cooper pairing *per se* as the background of superconductivity in MgB_2 is beyond question, as stems from the existence of the Josephson effect in break junctions [12]. Moreover, coherent peaks in the optical conductivity [13] and spin–lattice relaxation [14] (the latter results were disputed in Ref. 15) are indicative of conventional Bardeen–Cooper–Schrieffer (BCS) s-wave pairing in MgB_2. Nevertheless, the low-temperature (low-T) properties of MgB_2 deserve further attention, since genuine BCS-like asymptotics of various quantities are never observed. The situation resembles that for high-T_c oxides, where a predominantly $d_{x^2-y^2}$-wave symmetry of the superconducting order parameter is inferred both from phase-sensitive experiments and phase-insensitive ones, including measurements of low-T asymptotics [16]. However, it was shown earlier that the power-law behavior of the electronic contribution to the heat capacity $C(T)$, thermal conductivity, NMR spin–lattice relaxation, ultrasound attenuation, or magnetic field penetration depth may be equally well explained by the spatial averaging of these quantities over a random spatial distribution of superconducting domains with different T_c's and energy gaps [17–19]. This analysis was qualitative, and to describe the diverse experimental data for MgB_2 a more rigorous quantitative approach has been developed and is given below.

Before proceeding further to the model, it is necessary to give a short summary of the measurements of different properties appropriate to MgB_2 with a special emphasis on the inferred electron spectrum gapping in the superconducting state.

The low-T asymptotics of the magnetic field penetration depth $\lambda(T)$ was shown by muon spin-rotation [20], microwave surface resistance [21], and optical [13] measurements to be a power-law one. This was interpreted as either unconventional superconductivity or at least as a highly anisotropic *s*-wave pairing. On the other hand, resonant technique investigations of MgB_2 wires [22] and *c*-axis oriented films [23] revealed the exponential decrease of the T-dependent term $\Delta\lambda(T)$ in $\lambda(T)$, with the pertinent superconducting energy gap $\Delta(T)$ much smaller than is required by the weak-coupling BCS theory in view of the large resistively determined T_c of the substance. Actually, similar results were obtained by muon spin-rotation [24], mutual inductance [25], and resonance [26–28] techniques. Nevertheless, those authors ascribed the apparent deviations from the BCS theory to a two-gap character of superconductivity in MgB_2. We should stress that those experiments, giving averaged quantities, can not justify *precisely* this scenario, although clearly indicating that a simple conventional description is not adequate. As for the improvement of fitting on the basis of the two-gap approximation, its merits should be considered with caution too, since in this case at least two extra free parameters are added. On the other hand, $\lambda(T)$ measurements are particularly sample-dependent [29,30], which is very important for the interpretation. Namely, a single-coil mutual inductance technique showed [29,30] that for sintered pellets $\Delta\lambda(T) \propto T^2$, whereas for thin films $\Delta\lambda(T) \propto \propto \exp(-\Delta_L/T)$, with Δ_L reduced in comparison with the BCS-inferred value (the Boltzmann constant $k_B = 1$). Alternatively, the data for bulk samples of MgB_2 can be fitted well by the superposition of two *s*-wave-gap contributions, previously used to describe properties of $YBa_2Cu_3O_{7-y}$ [31]. The authors of Refs. 29, 30 also make the important point that the magnitudes of $\lambda(0)$ and the $\lambda(T)$ curves near T_c differ substantially for samples made in the same batch.

The results of thermoelectric power $S(T)$ studies reveal the complexity of the electronic properties of MgB_2. In Ref. 32 measurements of $S(T)$ and the resistivity $\rho(T)$ of $Mg_{1-x}Al_xB_2$ above T_c were carried out, and a predominately hole character of the current carriers was found, the deviations from linearity at higher temperatures being attributed to the electron-like sheets of the Fermi surface (FS). The existence of both holes and electrons in MgB_2 with a considerable change of transport properties above 150 K also follows from the $S(T)$ measurements carried out in Refs. 33–35. The thermal conductivity $\kappa(T)$ in polycrystalline samples of MgB_2 shows a superconducting gapping below T_c [33], apparently with smaller Δ than is consistent with the weak-coupling BCS value. On the other hand, experiments on single crystals [36], followed by the subsequent subtraction of the lattice term $\kappa_{ph}(T)$ from the overall $\kappa(T)$, led those authors to the conclusion that the electronic part $\kappa_{el}(T)$ of the thermal conductivity is fitted well by a combination of two BCS-like terms with smaller and larger gaps, $\Delta_S(0) = 1.65$ meV and $\Delta_L(0) = 5.3$ meV.

The optical data are more ambiguous than their transport counterparts. Specifically, in the infrared reflectance [37,38], transmission [39,40], and Raman [41] spectra only one *s*-wave-like superconducting gap manifests itself. It also turns out that the quasiparticle scattering rates τ^{-1} strongly exceed the relevant Δ amplitudes, so that the dirty limit is achieved (the Planck's constant $\hbar = 1$). This is at variance with estimates of the mean free path l from transport phenomena [42–44], according to which MgB_2 is a well-defined clean superconductor. High-resolution photoemission studies [45] also found one isotropic gap with $\Delta(T = 15\,\text{K}) \approx \approx 4.5$ meV and a T dependence of the BCS type.

Other Raman [46], optical transmission [47] and reflectance [47,48] measurements, as well as photoemission studies [49], testify that a two-gap description in this case is more adequate than a conventional one, involving a single gap. In Ref. 38 it is concluded that the single gap $\Delta \approx 1.5$–2 meV found there is a minimal value of the anisotropic gap covering the multi-sheet FS of MgB_2 .

Thermodynamic measurements might be decisive in determining the low-T symmetry-based superconducting properties of MgB_2 because the minority phases or grain boundaries do not affect the results substantially, in contrast to transport phenomena, for example. The behavior of the electronic heat capacity $C(T)$ near T_c is also of great importance for elucidating the nature of superconductivity here. And, indeed, there have been many specific heat investigations for MgB_2 performed by various groups [50]. Unfortunately, the isolation of the current-carrier contribution to the overall heat capacity is obscured by (i) phonon anharmonicity, (ii) the involvement of low-T Einstein optical modes, especially for compounds containing light elements, (iii) the Schottky term due to paramagnetic impurities, and (iv) the complex electronic band structure of MgB_2, leading to at least two important electron-DOS-driven terms [51]. In this connection, it should be stressed that although the *two-band* approximation involving two Sommerfeld constants γ_S [51] turns out to be a satisfactory fitting procedure, it cannot be true from a fundamental point of view because an almost continuous set of energy gaps is observed in different point-contact spectra of the *same* polycrystalline MgB_2 pellet for varying locations of the Pt needle [52]. Such apparently random distribution of gaps has been observed, e.g., in the tunneling spectra of Nb_3Sn [17,53].

The main features of the data for $C(T)$ are (i) small values of the phase transition anomaly $\Delta C = C_s - C_n$ at T_c [50,54–56] in comparison to the BCS case [57], when the ratio

$$\mu = \frac{\Delta C}{\gamma_S(T_c)T_c} \tag{1}$$

is equal to

$$\mu_{BCS} = \frac{12}{7\zeta(3)} \approx 1.43\ ; \tag{2}$$

and (ii) deviations from the asymptotic BCS behavior at $T << T_c$,

$$C_s^{\text{asympt}}(T) = N(0)\left(\frac{2\pi\Delta_0^5}{T^3}\right)^{1/2} \exp\left(-\frac{\Delta_0}{T}\right) . \tag{3}$$

Here the subscripts s and n correspond to the superconducting and normal states, respectively, $N(0)$ is the electron DOS at the Fermi level, and Δ_0 is the energy gap value at $T = 0$. As indicated above, for MgB_2 it is necessary to take into account a possible T dependence of the Sommerfeld «constant». The deviations from Eq. (3) may be twofold: power-law-like $\propto T^2$ [54] and of the form $\propto \exp(-A/T)$ [56,58,59], where the constant A is much less than $(\pi/\gamma)T_c \approx 1.76T_c$, the value inherent to the weak-coupling superconductor [57], and $\gamma = 1.7810\ldots$ is the Euler constant. Thus, the raw specific heat data do not give definite answers to the problems of the order parameter symmetry and the underlying mechanisms of superconductivity.

In this article, on the basis of the experimentally proved *distribution* of energy gaps we show that *both* main features of the bulk property $C_s(T)$ can be explained by the conventional s-wave superconductivity, so that these data can be easily reconciled with other observations [13,14]. The adopted approach, being an outgrowth of the earlier one [17–19], is phenomenological because the origin of the gap distribution is not known precisely. However, in accordance with the tunneling data [60], the gap distribution is considered to occur *in real space* rather than in **k** space, as was suggested, e.g., in Refs. 50, 54. The theoretical description of such spatially disordered superconductors depends on the ratio between the characteristic superconducting domain size L and the coherence length ξ [61]. If $L > \xi$, the superconducting properties are determined by local values of the order parameter Δ. Our approach corresponds to these so-called large-scale inhomogeneities, whereas the small-scale inhomogeneities correspond to the reverse inequality $L < \xi$ [62,63]. The quantity ξ is T-dependent and tends to infinity at T_c. Hence, in the close vicinity of T_c, strictly speaking, all inhomogeneities become small-scale ones, and a divergent correction proportional to $(T_c/T - 1)^{-1/2}$ appears in the expression for $C_s(T)$ [62]. Nevertheless, it can be easily shown that for conventional superconductors including MgB_2 the relevant T range is very small, so that its influence on the phase transition smearing is negligible. Moreover, it has been disclosed recently that the correction for three-dimensional superconductors is actually finite [63]. Therefore we can identify ξ with the T-independent coherence length, dependent on the Pippard coherence length $\xi_0 \approx v_F/\pi\Delta$ and the mean free path l [57]. Here v_F is the Fermi velocity. For MgB_2, which can be considered a clean superconductor [42,44], the quantities of interest are $\xi \approx \xi_0 << l \approx 600$ Å, although there is a significant scatter of the values of ξ_0 inferred from different experiments and for *different kinds* of samples [6,64], so that we may estimate this quantity as lying in the range from 25 to 120 Å. This dispersion of ξ_0 qualitatively correlates with the broad spectra of gaps in tunnel and point-contact spectra [6,50,52,60].

A competitive theory [65–72] was put forward to reconcile the numerous transport, optical, microwave, and thermodynamic experimental data and the almost obvious *s*-wave and phonon-driven character of superconductivity in MgB_2 . It is based on the idea of multi-gap superconductivity with the gap diversity on the different sheets of the Fermi surface, i.e., in momentum **k** space. This is an extension of the well-known two-band superconductivity concept [73], which, in turn, approximates the complex anisotropy of the electron spectrum in MgB_2 [6,74–77]. A more direct version of the anisotropic *s*-wave superconductivity in MgB_2 has also been considered [78,79].

The expected observable results of our theory and the two-band model differ in the sense that in the latter case there should be two different gap parameters connected by interband scattering matrix elements or gaps clustered into two groups [68]. On the other hand, we suggest that the gap distribution should be quasi-continuous due to the proximity effect. Since our theory is phenomenological, it may be also directly applied to other substances, including cuprates. This will be done in subsequent publications.

2. Theory

Let us examine a T-independent configuration of mesoscopic domains, with each domain having the following properties:

(A) at $T = 0$ it is described by a certain superconducting order parameter $\Delta_0 \le \Delta_0^{\max}$;

(B) up to a relevant critical temperature $T_{c0}(\Delta_0) = (\gamma/\pi)\,\Delta_0$, it behaves like an isotropic BCS superconductor, i.e., the superconducting order parameter $\Delta(T)$ is the Mühlschlegel function $\Delta(T) = \Delta_{BCS}(\Delta_0, T)$ [57]; and the electronic specific heat is characterized in this interval by the function $C_s(\Delta\, T)$;

(C) at $T > T_{c0}$ it transforms into the normal state, and the relevant property is $C_n(T)$.

At the same time, the values of Δ_0 scatter for different domains. The current carriers move freely across domains and acquire appropriate properties inside each domain. The adopted picture is especially suitable for superconductors with small coherence lengths ξ_0 [50], where even nanoscale intrinsic inhomogeneities may comprise domains of the sort discussed above.

In other words, each domain above its T_{c0} is in the normal phase, and its specific heat is [57]

$$C_n(T) = \frac{\pi^2}{3} N(0) T \ . \tag{4}$$

For simplicity we restrict ourselves to the situation when the whole sample above T_c is electronically homogeneous, i.e., is characterized by a common, approximately constant $N(0)$ value. Below T_{c0} for a given mesoscopic domain, a corresponding isotropic gap appears on the Fermi surface. The microscopic background of the assumed scatter in T_{c0} may be diverse but ultimately manifests itself as a variation either of the magnitude of the electron–phonon interaction or of the local values of the Coulomb pseudopotential.

In the framework of our phenomenological approach, superconductivity (if any) inside a chosen domain is described by the relevant parameters Δ_0 and T_{c0}. They are bounded from above by $\Delta_0^{\max}$ and T_c, respectively. These Δ_0 may or may not group around a certain crowding value Δ_0^*, depending on the sample texture. The existence of such two possibilities is in accordance with the varied data for MgB_2 [6,50–52,60]. The specific gap distribution is described by the function $f_0(\Delta_0)$.

Thus, for all T in the interval $[0, T_c]$, where $T_c = \max T_{c0}$, the superconducting sample consists of superconducting (s) and nonsuperconducting (n) grains more or less homogeneously distributed over the sample volume. The critical temperature T_c defined in such a manner may not necessarily coincide with the resistively determined T_c^{res} governed by percolation networks in the disordered samples [80,81].

The measured $C_s(T)$ is an averaged sum of contributions from both phases,

$$\langle C(T)\rangle = \langle C_n(T)\rangle + \langle C_s(T)\rangle \ , \tag{5}$$

which depends on the distribution function $f(\Delta, T)$ of superconducting domains and on the normal-phase fraction $\rho_n(T)$ [17–19]:

$$\langle C_n(T)\rangle = C_n(T)\rho_n(T) \ , \tag{6}$$

$$\langle C_s(T)\rangle = \int_0^{\Delta^{\max}(T)} C_s(\Delta, T) f(\Delta, T)\, d\Delta . \tag{7}$$

Here $\Delta^{\max}(T) = \Delta_{BCS}(\Delta_0^{\max}, T)$, and $f(\Delta, T)$ is a result of the thermal evolution of the initial (at $T = 0$) distribution function $f_0(\Delta_0)$.

It is convenient to normalize all temperatures by T_c and all energy parameters by $\Delta_0^{\max}$:

$$t = T/T_c, \quad \delta = \Delta/\Delta_0^{\max} \ , \tag{8}$$

with relevant indices retained, and to consider $C_s(T)$ and $C_n(T)$ together with their averaged counterparts, normalized by the $C_n(T_c)$ value, i.e., for example,

$$c_{s,n}(t) = \frac{C_{s,n}(T)}{C_n(T_c)} . \tag{9}$$

Then one can easily find that for each domain, characterized by the parameter δ_0 at $t = 0$, the dimensionless heat capacity is either

$$c_n(t) = t \quad \text{for} \quad t > \delta_0 \tag{10}$$

or

$$c_s(t) = \delta_0 c_{BCS}\left(\frac{t}{\delta_0}\right) \ \text{for} \ \ t < \delta_0 , \tag{11}$$

where $c_{BCS}(x)$ is a well-known normalized heat-capacity function for a standard BCS superconductor [57]. The parameter $N(0)$, due to the assumption $N(0) = \text{const}$, disappears from the normalized dependences (10) and (11).

For a surmised domain ensemble a distribution function $f(\Delta, T)$ for finite T is defined by the formula

$$f(\Delta, T)\, d\Delta = f_0(\Delta_0)\, d\Delta_0 . \tag{12}$$

Then Eq. (7) can be rewritten as

$$\langle c_s(t)\rangle = \int_t^1 c_{BCS}\left(\frac{t}{\delta_0}\right) f_0(\delta_0)\, \delta_0\, d\delta_0 . \tag{13}$$

To obtain the low-T asymptotics, we introduce a new integration variable $z = t/\delta_0$. Then,

$$\langle c_s(t)\rangle = t^2 \int_t^1 \frac{dz}{z^3} f_0\left(\frac{t}{z}\right) c_{BCS}(z) . \tag{14}$$

Expanding the function $f_0\left(\frac{t}{z}\right)$ into a series

$$f_0\left(\frac{t}{z}\right) = f_0(0) + \sum_{k=1}^{\infty} B_k \left(\frac{t}{z}\right)^k , \tag{15}$$

we arrive at

$$\langle c_s(t)\rangle = t^2 f_0(0) \int_0^1 \frac{dz}{z^3} c_{BCS}(z) + t^2 \left[- f_0(0) \int_0^t \frac{dz}{z^3} c_{BCS}(z) + \sum_{k=1}^{\infty} B_k t^k \int_t^1 \frac{dz}{z^{k+3}} c_{BCS}(z) \right] . \tag{16}$$

The first term in the right-hand side is the sought asymptotics

$$\langle c_s(t \to 0)\rangle = t^2 f_0(0) \int_0^1 \frac{dz}{z^3} c_{BCS}(z) \approx 2.45 f_0(0)\, t^2 . \tag{17}$$

Note that in our previous works [17–19], to estimate the numerical coefficient in the asymptotic term we used the dependence $C_s^{\text{asympt}}(T)$ instead of $C_{BCS}(T)$, which led to the result $\langle c_s(t \to 0)\rangle \approx \approx 0.54\, f_0(0)\, t^2$.

The dependence of the next term in the expansion for $\langle c_s(t)\rangle$ can be estimated in the limit $t \to 0$ by substitution of the normalized expression (3) for $c_{BCS}(z)$. Then

$$\int_0^t \frac{dz}{z^3} c_{BCS}(z) \approx \frac{3\sqrt{2}\gamma}{\pi^2 \sqrt{\pi}} \Gamma\left(\frac{7}{2}, \frac{\pi}{\gamma t}\right) . \tag{18}$$

For small t this expression decreases as $O[t^{5/2} \exp(-\pi/\gamma t)]$. At the same time, the convergence of the series in Eq. (16) for $t \to 0$ is $O(t^4)$ if the function $f_0(\delta_0)$ has an extremum at $\delta_0 = 0$ (then the coefficient $B_1 = 0$), or $O(t^3)$ otherwise.

Now, in the same low-T region let us take a look at the contribution $\langle c_n(t)\rangle$ of the continuously expanding normal phase. At any T, all domains with $\Delta_0 < (\pi/\gamma)\, T$ (i.e., $\delta_0 < t$) are nonsuperconducting, with the total normal-phase fraction being

$$\rho_n(t) = \rho_n(0) + \int_0^t f_0(\delta_0)\, d\delta_0 . \tag{19}$$

For simplicity, below we restrict ourselves to the case when all domains at $t = 0$ are superconducting, i.e., $\rho_n(0) = 0$. The generalization to the case $\rho_n(0) \neq 0$ is obvious: at each temperature there exists an additional contribution from the normal phase. Then the function $f_0(\delta_0)$ should be normalized by $1 - \rho_n(0)$, and all averaging-driven effects would accordingly decrease. Moreover, if $\rho_n(0) \neq 0$, the observed heat capacity $\langle c(t)\rangle$ must include an extra linear contribution $\rho_n(0)t$ in the true superconducting state exhibiting the Meissner effect. On the other hand, the observation of the resistive macroscopic superconductivity depends on the crossing of the percolation threshold by the superconducting domain fraction.

As to the second term in Eq. (19), the approximation of $f_0(\delta_0)$ by its limiting value $f_0(0)$ demonstrates that the main temperature-dependent contribution to $\rho_n(t)$ is *linear* in t. Since $c_n(t)$ is also a linear function of t, the apparent contribution $\langle c_n(t)\rangle$ of the normal phase to the total specific heat $\langle c(t)\rangle$ is quadratic in t for small t, similarly to

$\langle c_s(t)\rangle$. Thus, in the proposed model of a disordered superconductor with a broad continuous spatial distribution of domains possessing different T_{c0}'s, the normal and superconducting contributions to thermodynamic quantities are *functionally indistinguishable* from each other.

3. Numerical results

In addition to the low-T asymptotics the overall T dependence of the heat capacity C up to T_c is also of considerable interest. It is especially important to trace the smearing of the anomaly ΔC by the *same* disorder effect that leads to the transformation of the intrinsic exponential low-T behavior of $C_s(T)$ into power-law behavior. These objectives were met by numerical calculations.

For this purpose, two model distribution functions $f_0(\delta_0)$, namely, exponential

$$f_0^E(\delta_0) \propto \exp\left[-\frac{|\delta_0-\delta_0^*|}{d}\right] \tag{20}$$

and Gaussian

$$f_0^G(\delta_0) \propto \exp\left[-\frac{(\delta_0-\delta_0^*)^2}{2d^2}\right] \tag{21}$$

were used. The parameter δ_0^* designates the peak position, which may vary from 0 to 1. By changing the parameter d we control the dispersion of the domain superconducting properties: the sharper the function $f_0(\delta_0)$, the more homogeneous the ensemble. Nevertheless, for any d both functions are nonvanishing in the limit $\delta_0=0$ and their Taylor series (15) begin with the relevant constants as the main terms. Only for highly improbable distribution functions such that $f_0(\delta_0)$ extends to $\delta_0=0$ and also satisfies the condition $f_0(\delta_0=0)=0$ can the Taylor series begin with the next term, resulting in the asymptotics $C_s(T)\propto T^3$.

Figure 1 shows the influence of the choice of distribution function on $\langle c_s(t)\rangle$ for $\delta_0^*=1$ (*a*) and $\delta_0^*=0$ (*b*). In all cases, for larger d the curves converge towards a common limit which corresponds to the uniform distribution $f_0^U(\delta_0)=\text{const}$. For smaller d the curves approach opposite homogeneous bounds: the discontinuous curve for a clean BCS superconductor (Fig. 1,*a*) and the straight line, coinciding with the abscissa, for a normal metal (Fig. 1,*b*). Thus, on Fig. 1,*b* the curves become more and more flat. As to Fig. 1,*a* even for $d=0.1$ [i.e., when $f_0(0)/f_0(1)\approx 4.5\cdot10^{-6}$ for the exponential distribution and $\approx 1.9\cdot10^{-22}$ for the Gaussian] the resulting curves are no longer discontinuous: the jump transforms into a hump. In addition, with variation of the parameter d the peak positions on the two panels shift in opposite directions.

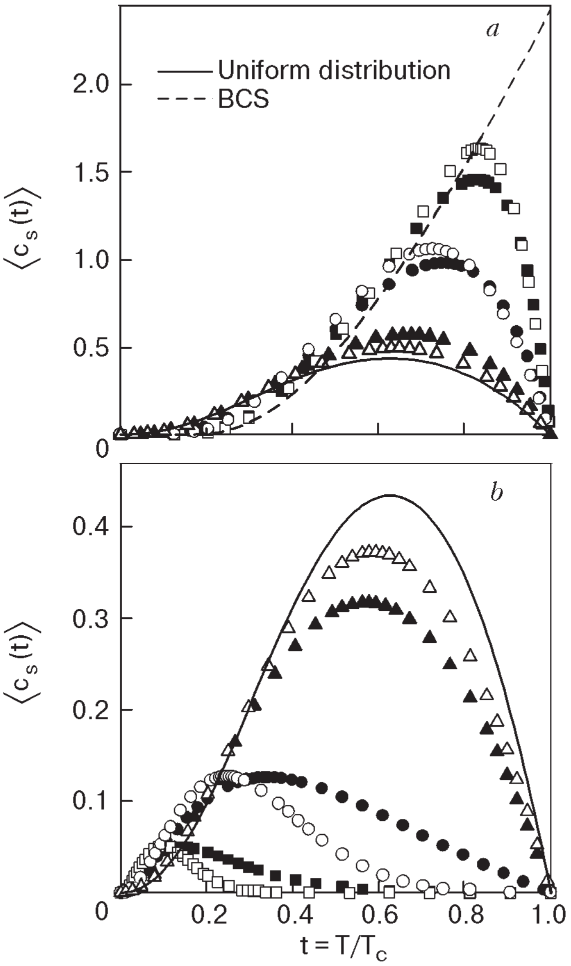

Fig. 1. Temperature dependences of normalized (see the text) electronic heat capacity $\langle c_s(t)\rangle$ of superconducting phase fraction for exponential and Gaussian distributions of the parameter δ_0 over the inhomogeneous ensemble of domains. The panels correspond to the maximum position at $\delta_0^*=1$ (*a*) and $\delta_0^*=0$ (*b*). For $d=0.1$ — exponential (■), Gaussian (□); $d=0.25$ — exponential (●), Gaussian (○); $d=1$ — exponential (▲), Gaussian (△).

Thus, the substantial spreading of the anomaly ΔC readily seen in Fig. 1 seems quite natural in view of the results for MgB_2 [50,54–56]. However, the concomitant superposition of various domain contributions causes distortion of the overall curves $C_s(T)$ and $C(T)$, which is much less trivial. This very superposition may lead for low T to the power-law behavior whose the asymptotics was analyzed above.

Figure 1 also evidences that different distributions lead to similar results for each set of parame-

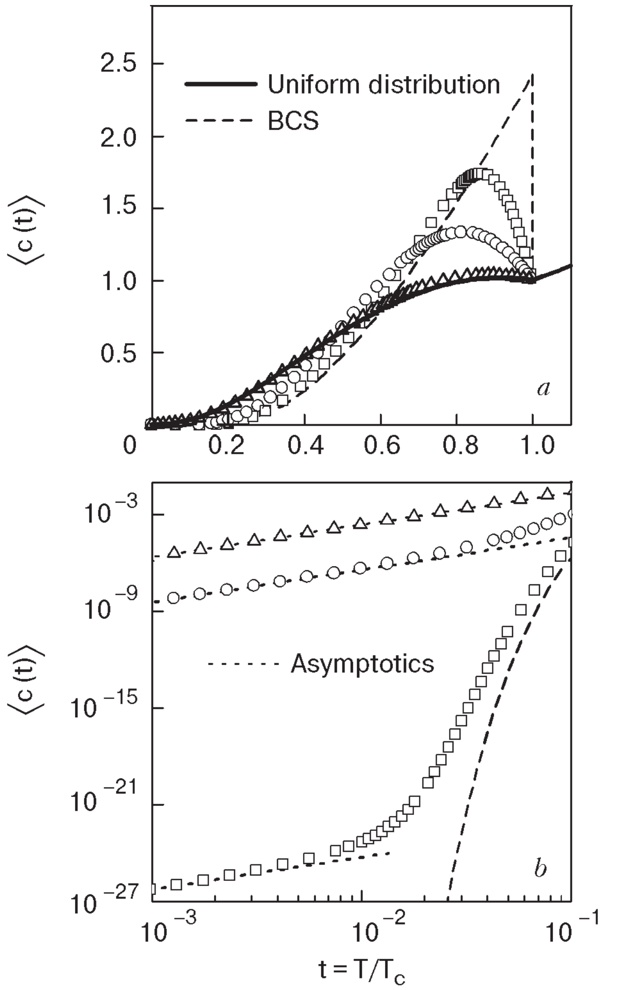

Fig. 2. Temperature dependences of normalized total electronic heat capacity $\langle c(t)\rangle$ in comparison with the BCS dependence of the superconducting-phase fraction. Gaussian distributions with $\delta_0^* = 1$ (*a*). Low-temperature portions of the relevant curves on a log–log scale together with their t^2 asymptotics (*b*). For $d = 0.1$ (□), $d = 0.25$ (○), $d = 1$ (△).

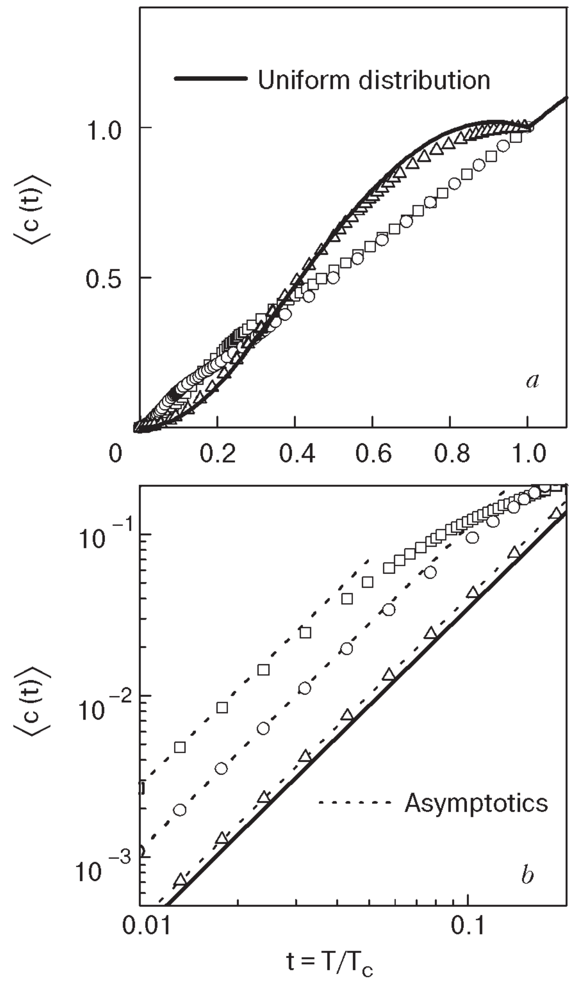

Fig. 3. Temperature dependences of normalized total electronic heat capacity $\langle c(t)\rangle$ for Gaussian distributions with $\delta_0^* = 0$ (*a*). Low-temperature portions of the relevant curves on a log–log scale together with their t^2 asymptotics (*b*). For $d = 0.1$ (□), $d = 0.25$ (○), $d = 1$ (△).

ters, and it would be the more so if we plotted the relevant $\langle c(t)\rangle$ curves. Hence, hereafter we confine ourselves to the Gaussian distribution.

The dependences $\langle c(t)\rangle$ are depicted in the Fig. 2,*a* for $\delta_0^* = 1$ and different dispersion values *d*. The low-*T* parts of the $\langle c(t)\rangle$ curves are displayed on a log–log scale in Fig. 2,*b*. The dotted straight lines correspond to the pertinent T^2 asymptotics for each curve. It is clear that the validity range of the asymptotics extends with the increase of *d*. Although intervals where the T^2 approximation holds good exist for any *d*, for small *d* this is merely of academic interest, because both temperatures and heat capacities become too tiny to be experimentally significant. On the other hand, for higher *T* in this case the averaged curves $\langle c(t)\rangle$ lie rather close to the exponential curve inherent to the BCS theory (the dashed curve). Such transitional parts of the dependences $\langle c(t)\rangle$ describe well the exponential low-*T* behavior for some samples of MgB_2 [56,58] with smaller exponents than in the BCS case.

For large *d*, when the Gaussian distribution function $f_0^G(\delta_0)$ becomes almost uniform (such a random dense, although quasi-discrete, distribution of gaps was found in point-contact spectra [52]), the quadratic asymptotics are valid at least up to $t = 0.1$ (for the uniform distribution $f_0^U(\delta_0)$ the relative error of the t^2 asymptotics is $\approx 0.6\%$ at $t = 0.1$ and $\approx 5\%$ at $t = 0.2$), which agrees with the measurements [54]. For intermediate *d* the experimental

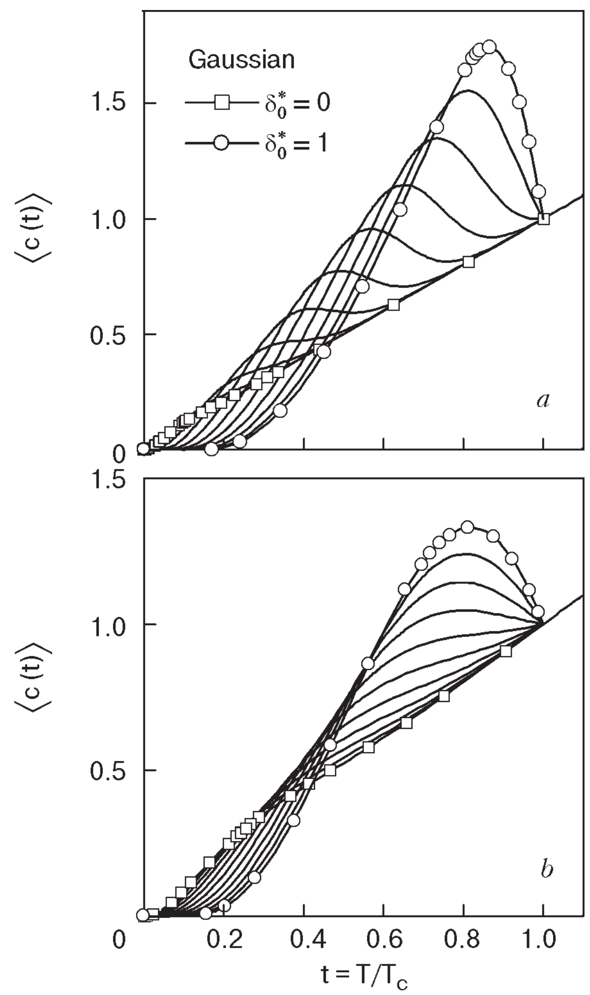

Fig. 4. Influence of the peak position δ_0^* in the Gaussian distribution function on the behavior of $\langle c(t)\rangle$. Dispersion $d = 0.1$ (*a*) and $d = 0.25$ (*b*). δ_0^* varies from 0 to 1 in steps of 0.1.

data in the relevant T range may be satisfactorily represented by power-law curves $C(T) \propto T^n$ with $n \geq 2$.

Figure 3 demonstrates the dependences $\langle c(t)\rangle$ for $\delta_0^* = 0$. The overall behavior remains the same as for $\delta_0^* = 1$, but the validity range of the asymptotics extends because now $f_0(\delta_0)$ has a maximum at $\delta_0 = 0$, in full agreement with the analysis given above (see Sec. 2).

One can make another important conclusion from the numerical data shown in Figs. 2 and 3. Specifically, a one-parameter fitting explains *both* the smearing of the heat-capacity anomaly at T_c and the appearance of the power-law asymptotics. The latter reproduces the results appropriate to superconductors with order parameters of $d_{x^2-y^2}$-wave [82] or extended *s*-wave with uniaxial anisotropy [50,54] symmetry. The patterns displayed in these figures explain well the experimental heat capacity dependences $C(T)$ for MgB_2, which demonstrate power-law behavior for lowest attainable T [50,54] or above the exponential low-T tail [58]. At the same time, the reduction of the anomaly ΔC at T_c with the increase of d, traced in Fig. 2,*a*, adequately describes the ΔC magnitudes inferred from the analysis of the observed total heat capacity of MgB_2, with allowance made for the crystal-lattice and impurity components. Namely, $\mu \approx 1.13$ [56], 0.82 [50,54], 0.7 [55], so that the experimental specific heat jump is substantially smaller than the BCS value μ_{BCS} (see Eq.(2)).

A comparison of Figs. 2,*a* and 3,*a* shows that for wide enough distribution functions the resulting $\langle c(t)\rangle$ curves are almost identical. They lie very close to the corresponding curve for the uniform distribution. The latter has a gentle maximum at about $t = 0.9$, so that the actual t dependence in the interval $0.8 \leq t \leq 1$ may be readily overlooked. It is clear that the peak position δ_0^* has no meaning in this case. At the same time, for small d, if the parameter δ_0^* changes from 1 to 0, the curves transform from ones possessing well-pronounced maxima to almost monotonic ones. Such a transformation «process» is depicted in Fig. 4. In particular, the results show an interesting feature: if the distribution over Δ_0 is characterized by a small dispersion and a maximum position at about $\Delta_0^{\max}/2$, the apparent dependence $\langle C(T)\rangle$ should demonstrate «oscillating» behavior in the superconducting temperature region. For example, for $d = 0.1$ it would happen above $t \approx 0.4$, according to Fig. 4,*a*. These departures from the BCS electronic specific heat describe qualitatively the deviations of the experimental $C(T)$ from their counterparts measured in strong magnetic fields, when superconductivity is suppressed [51,54,55].

4. Discussion and conclusions

The results obtained here are of a quite general nature and fit well the observed heat capacity dependencies both for cuprates and magnesium diboride. Our main assumptions are the *s*-wave symmetry of the superconducting order parameter and the proposed large scale ($L > \xi_0$) spatial inhomogeneities of Δ (and T_c). As for cuprates, the origin of those heterogeneities was discussed in our previous publications [17,18]. On the other hand, in MgB_2 large enough inclusions (they influence the heat capacity!) of different phases or planar defects may be the most probable cause of the Δ spread. One can mention, e.g., observed MgB_4 grains and stacking faults [83] or nonstoichiometry modeled by $Mg_{1+\delta}B_2$ phases [84]. Mg vacancies or B interstitials as well as some degree of oxidation may be the inhomogeneities leading to conspicuous scatter of T_c [85]. X-ray analysis shows that MgB_2 can be microscopically nonstoichiometric up to 5–10% [86]. Nonstoichiometry is most likely an intrinsic phenomenon, since pressure dependences of T_c are substantially different for various specimens [10,87]. However, we can not also exclude a purely electronic phase separation [81,88–94], because the substance concerned is on the verge of an electronic topological transition [74,77,95] or a structural one [87,96].

Bearing in mind these inhomogeneities of sintered, single-crystal, and thin-film MgB_2 samples, we applied our theory to calculate the spatially averaged electronic heat capacity $\langle C(T)\rangle$. The low-T asymptotics was shown to be a power-law one $\propto T^2$, the anomaly ΔC at T_c being simultaneously smeared. These very features are appropriate to the heat capacity of MgB_2. The existence of regions (domains) with varying T_c undoubtedly manifests itself in the photoemission, Raman, point-contact, and tunneling spectra [6,46,49,52,60, 97–104]. Usually the two-gap description is sufficient to fit the observations, but we should stress that it may be only a crude approximation of the actual really *multiple-gap* picture. For example, a three-gap structure was also seen in the *same* tunneling spectrum [105].

We suggest that the observed multiple-gap superconductivity in MgB_2 originates from some kind of a phase separation or an intrinsic nonstoichiometry rather than from the existence of several groups of current carriers in the same volume [65–68,70,72]. The proposed theory may be also invoked to explain the low-T properties of cuprates [17–19], although the microscopic background of the multi-gapness may be quite different in both cases.

One more circumstance should be highlighted to distinguish between various scenarios of apparent two-gap (or, better to say, multiple-gap) manifestations. It is often claimed [49,98] that for MgB_2 both gaps close at a *common* T_c. But even a cursory examination of the relevant data shows that the instrumental errors in the neighborhood of T_c and the obvious uncertainties of applied fittings are too large to ensure the validity of such a conclusion. Indeed, some point-contact spectra could be explained on the basis of two gaps, one vanishing at the bulk T_c while the other closing at $\approx 0.7\,T_c$ [52]. Also the differential conductivities of MgB_2/Ag and MgB_2/In junctions have been interpreted in terms of two gaps with energies 4 and 2.6 meV, which close at 20 and 38 K, respectively [99]. This alleged anticorrelation between the Δ's and T_c's seems doubtful and apparently is a consequence of the two-gap prescription. On the other hand, the experimental results [49,98,99] can be naturally described in the framework of the scheme adopted here with a continuous set of gaps and critical temperatures rigidly bound to them. Hence, the two-gap fitting procedure is only a first approximation to the actual multiple gap superposition. Aside from the formal aspect of the problem consisting in the selection of a proper fitting procedure, our point of view is favored by the direct simultaneous experimental observations of more than two gaps for a number of samples [52,60].

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