Why Magnesium Diboride Is Not Described by Anisotropic Ginzburg-Landau Theory

A. E. Koshelev[1] and A. A. Golubov[2]
[1]*Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439, USA*
[2]*Faculty of Science and Technology, University of Twente, 7500 AE Enschede, The Netherlands*
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It is well established that the superconductivity in the recently discovered superconducting compound MgB_2 resides in the quasi-two-dimensional band (σ band) and three-dimensional band (π band). We demonstrate that, due to such band structure, the anisotropic Ginzburg-Landau theory practically does not have a region of applicability, because gradient expansion in the c direction breaks down. In the case of a dirty π band, we derive the simplest equations, which describe properties of such superconductors near T_c, and explore some consequences of these equations.

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Ginzburg-Landau (GL) theory is the most powerful and widely used phenomenological theory of superconductivity (see, e.g., Refs. [1,2]). It describes practically all known superconductors in the vicinity of transition temperature. GL theory is fully microscopically justified and all its parameters can be derived from the microscopic BCS theory [3]. GL theory provides the basis for such elaborated fields as vortex physics [4] and the theory of fluctuation phenomena [2].

The recently discovered superconductor MgB_2 [5] gives an example of a superconductor which *is not described by the anisotropic GL theory*. This very unusual feature is a consequence of a specific band structure of this compound. It is reliably established that superconductivity in MgB_2 resides in two families of bands: strongly superconducting quasi-two-dimensional σ bands and weakly superconducting three-dimensional π bands (see, e.g., Ref. [6]). Both bands are characterized by their intrinsic coherence lengths, and the c axis coherence length in the σ band is much smaller than c axis coherence length in the π band. Typically, the strong band forces the order parameter in the weak band to change in the c direction at distances smaller than the intrinsic c axis coherence length in this band. This means that almost in the whole temperature range the effective coherence length in the c direction, $\xi_z(T)$, is smaller than the intrinsic coherence length in the π band, $\xi_{\pi,z}$. The crossover to the GL region takes place only when $\xi_z(T)$ exceeds $\xi_{\pi,z}$, which occurs in the very close vicinity of T_c. In this narrow region the π band strongly increases the c axis coherence length. Beyond the narrow region, the variations of the order parameter in the c directions are not described by the anisotropic GL theory. Important consequences of GL theory breakdown are the strong temperature dependence of the H_{c2} anisotropy [7–10] and strong deviations of the H_{c2} angular dependence from the simple "effective mass" law [10,11].

Obviously, the breakdown of the anisotropic GL theory has numerous consequences and it would be desirable (i) to trace the reason of this breakdown and (ii) to derive the simplest model, which replaces the GL model near T_c. This Letter addresses these issues. For illustration, we use the simplest microscopic model, multiband generalization of the Usadel theory, describing a dirty two-band superconductor with weak interband scattering [9,12]. However, the main conclusions are very general and do not depend much on the intraband scattering strength. In the model we use the GL expansion for the σ band and keep the microscopic description for the π band, i.e., only "dirtiness" of the π band is essential for a particular form of equation.

We consider a dirty two-band superconductor with weak interband scattering. Such a superconductor is described by Usadel equations for the impurity averaged normal and anomalous Green's functions, G_α and F_α, $G_\alpha^2 + |F_\alpha|^2 = 1$, and the pair potentials Δ_α,

$$\omega F_\alpha - \sum_j \frac{\mathcal{D}_{\alpha,j}}{2}[G_\alpha D_j^2 F_\alpha - F_\alpha \nabla_j^2 G_\alpha] = \Delta_\alpha G_\alpha, \quad (1)$$

where $\alpha = 1, 2$ is the band index, $j = x, y, z$ is the coordinate index, $D_j \equiv \nabla_j - (2\pi i/\Phi_0)A_j$, $\mathcal{D}_{\alpha,j}$ are diffusion constants, and $\omega = 2\pi T(s + 1/2)$ are Matsubara frequencies. Bearing in mind the application to MgB_2, in our notations index 1 corresponds to σ bands and index 2 to π bands, $\mathcal{D}_{1,j} \equiv \mathcal{D}_{\sigma,j}$ and $\mathcal{D}_{2,j} \equiv \mathcal{D}_{\pi,j}$. All bands are isotropic in the xy plane and anisotropic in the xz plane with the anisotropy ratios $\gamma_\alpha = \sqrt{\mathcal{D}_{\alpha,x}/\mathcal{D}_{\alpha,z}}$. Self-consistency conditions can be written as [12]

$$W_1\Delta_1 - W_{12}\Delta_2 = 2\pi T \sum_{\omega>0}\left(F_1 - \frac{\Delta_1}{\omega}\right) + \Delta_1 \ln\frac{1}{t}, \quad (2a)$$

$$-W_{21}\Delta_1 + W_2\Delta_2 = 2\pi T \sum_{\omega>0}\left(F_2 - \frac{\Delta_2}{\omega}\right) + \Delta_2 \ln\frac{1}{t}, \quad (2b)$$

where $t \equiv T/T_c$ and the matrix $W_{\alpha\beta}$ is related to the matrix of coupling constants $\Lambda_{\alpha\beta}$ as

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$$W_1 = \frac{-\Lambda_- + \sqrt{\Lambda_-^2 + \Lambda_{12}\Lambda_{21}}}{\mathrm{Det}}, \qquad W_2 = \frac{\Lambda_- + \sqrt{\Lambda_-^2 + \Lambda_{12}\Lambda_{21}}}{\mathrm{Det}}, \qquad W_{12} = \Lambda_{12}/\mathrm{Det}, \qquad W_{21} = \Lambda_{21}/\mathrm{Det},$$

$\Lambda_- \equiv (\Lambda_{11} - \Lambda_{22})/2$, $\mathrm{Det} \equiv \Lambda_{11}\Lambda_{22} - \Lambda_{12}\Lambda_{21}$, $W_1 W_2 = W_{12}W_{21}$. The supercurrent components are given by

$$j_j = 4\pi eT \sum_\alpha \sum_{\omega>0} N_\alpha \mathcal{D}_{\alpha,j} \mathrm{Im}[F_\alpha^* D_j F_\alpha], \tag{3}$$

where N_α are the partial densities of states.

We start with the derivation of the GL equations from the Usadel equations in the close vicinity of T_c following a standard route. In the lowest approximation $G_\alpha^{(0)} = 1$ and $F_\alpha^{(0)} \approx \Delta_\alpha/\omega$. When Δ_α are small and change slowly in space (the exact criterion will be derived below) one can keep only the leading nonlinear and gradient corrections

$$F_\alpha \approx \frac{\Delta_\alpha}{\omega} - \frac{\Delta_\alpha^3}{2\omega^3} + \sum_j \frac{\mathcal{D}_{\alpha,j}}{2\omega^2} D_j^2 \Delta_\alpha. \tag{4}$$

Substituting this expansion into the self-consistency conditions (2), we obtain coupled GL equations for two gap parameters [13]

$$W_1\Delta_1 - W_{12}\Delta_2 = \sum_j \xi_{1,j}^2 D_j^2 \Delta_1 - b\Delta_1^3 + \tau\Delta_1, \tag{5a}$$

$$-W_{21}\Delta_1 + W_2\Delta_2 = \sum_j \xi_{2,j}^2 D_j^2 \Delta_2 - b\Delta_2^3 + \tau\Delta_2, \tag{5b}$$

with $\xi_{\alpha,j}^2 = (\pi/8T)\mathcal{D}_{\alpha,j}$, $b = 7\zeta(3)/(8\pi^2T^2)$ and $\tau = \ln(1/t) \approx (T_c - T)/T_c$.

Near T_c the right-hand sides of Eqs. (5) are small. This allows us to reduce Eqs. (5) to a single GL equation by looking for a solution for Δ_2 in the form

$$\Delta_2 \approx \frac{W_{21}}{W_2}\Delta_1 + \delta_2. \tag{6}$$

From Eqs. (5) we obtain

$$-W_{12}\delta_2 = \sum_j \xi_{1,j}^2 D_j^2 \Delta_1 - b\Delta_1^3 + \tau\Delta_1, \tag{7a}$$

$$W_2\delta_2 = \sum_j \xi_{2,j}^2 D_j^2 \Delta_2 - b\Delta_2^3 + \tau\Delta_2. \tag{7b}$$

The second equation indicates that δ_2 is a small correction, $\delta_2 \ll \Delta_2$, and one can use $\Delta_2 \approx (W_{21}/W_2)\Delta_1$ in the right-hand side of this equation. Excluding δ_2 and introducing the band-averaged order parameter

$$\Delta^2 = \frac{W_2\Delta_1^2 + W_1\Delta_2^2}{W_2 + W_1} \approx \frac{W_{12}W_2^2 + W_{21}W_1^2}{W_{12}W_2(W_2 + W_1)}\Delta_1^2,$$

we finally obtain the anisotropic GL equation for Δ

$$-\sum_j \xi_j^2 D_j^2 \Delta + b\Delta^3 - \tau\Delta = 0, \tag{8}$$

with the average coherence lengths

$$\xi_j^2 = \frac{W_2\xi_{1,j}^2 + W_1\xi_{2,j}^2}{W_2 + W_1}.$$

For the supercurrent, using relation $W_{21}/W_{12} = \Lambda_{21}/\Lambda_{12} = N_1/N_2$, we derive

$$j_j \approx 4eNP\xi_j^2 \mathrm{Im}[\Delta^* D_j \Delta], \tag{9}$$

with $N \equiv N_1 + N_2$ and

$$P \equiv \frac{N_1N_2(W_2 + W_1)^2}{(N_1 + N_2)(N_2W_2^2 + N_1W_1^2)}.$$

From Eqs. (8) and (9) we derive the components of the London penetration depth

$$\lambda_j^{-2} \approx \frac{32\pi^2 eNP\xi_j^2\tau}{c\Phi_0 b}.$$

For the parameters of MgB_2, $W_1 \ll W_2$, $\xi_{1,z} \ll \xi_{2,z}$, $\xi_{1,x} \sim \xi_{2,x}$, the dominating effect of the π band is the renormalization of the c axis lengths

$$\xi_z^2 \approx \xi_{1,z}^2 + S_{12}\xi_{2,z}^2, \tag{10}$$

$$\lambda_z^{-2} \approx \frac{32\pi^2 e\tau N_1}{c\Phi_0 b}(\xi_{1,z}^2 + S_{12}\xi_{2,z}^2), \tag{11}$$

with $S_{12} \equiv W_1/W_2 \ll 1$. The influence of the π band on properties not related with the variations of the order parameter along the c axis are weak and can be treated perturbatively.

We obtain now the applicability criterion for the GL expansion. The gradient expansion is justified if $-\xi_{\alpha,j}^2\nabla_j^2\Delta_\alpha < \Delta_\alpha$ for all α and i. Because a typical scale of the spatial variations is the temperature-dependent GL coherence length $\xi_j(T)$, this condition simply means

$$\xi_j(T) > \xi_{\alpha,j}. \tag{12}$$

The most restraining inequality is the one for $\alpha = 2$ and $i = z$, which gives

$$(T_c - T)/T_c < \xi_{1,z}^2/\xi_{2,z}^2 + S_{12}. \tag{13}$$

Because $\xi_{1,z} \ll \xi_{2,z}$ and $S_{12} \ll 1$, the applicability of the GL approach is limited to an extremely narrow temperature range near T_c; i.e., the situation is very different from conventional superconductors. For parameters of MgB_2 this condition implies $(T_c - T)/T_c \ll 0.05$. On the other hand, near T_c the fluctuation effects become important. This means that the mean-field GL theory practically does not have a region of applicability.

We derive now the simplest theory which replaces the GL theory in the conventional GL region $(T_c - T)/T_c < 1$. As the gradient expansion actually breaks down only for the π band, in the vicinity of T_c we can proceed with the expansion (4) for the σ band, $\alpha = 1$. Substituting this expansion into the self-consistency conditions, we obtain Eq. (5a). The π band only weakly renormalizes the nonlinear term and we can use the linear approximation in this band,

$$\omega F_2 - \sum_j \frac{\mathcal{D}_{2,j}}{2} D_j^2 F_2 = \Delta_2. \tag{14}$$

The π band order parameter can again be represented by Eq. (6) with δ_2 being a small correction. Finding this correction from Eq. (2b) and substituting it into Eq. (2a) together with the GL expansion for F_1, we derive coupled equations for Δ_1 and reduced π band F function f_s, $f_s \equiv (2\pi T W_2/W_{21})F_2(\omega_s)$ [14]

$$-(1+S_{12})\tau\Delta_1 + b\Delta_1^3 - \sum_j \xi_{1,j}^2 D_j^2 \Delta_1 - S_{12}\sum_{s=0}^{\infty}\left(f_s - \frac{\Delta_1}{s+1/2}\right) = 0, \tag{15a}$$

$$(s+1/2)f_s - \frac{2}{\pi^2}\sum_j \xi_{2,j}^2 D_j^2 f_s = \Delta_1, \tag{15b}$$

and the expression for the supercurrent

$$j_j \approx 4eN_1\xi_{1,j}^2 \mathrm{Im}[\Delta_1^* D_j \Delta_1] + \frac{8e}{\pi^2} N_1 S_{12}\xi_{2,j}^2 \sum_{s=0}^{\infty} \mathrm{Im}[f_s^* D_j f_s].$$

These equations replace the GL equations in the case of a dirty π band. Note that the same equations are also valid in the case of a clean σ band but with a different definition of the coherence length $\xi_{1,j}$, $\xi_{1,j}^2 = 7\zeta(3)\langle v_{1,j}^2\rangle/(4\pi T)^2$.

In the case of weak superconductivity in the π band, $S_{12} \ll 1$, and for $\xi_{1,z} \ll \xi_{2,z}$, one can neglect the in-plane gradients in Eq. (15b) and obtain an even simpler set of equations which describe only *the dominating strong effects*, related to inhomogeneities of the gap parameter along the c axis, and neglect small renormalizations of the coefficients by the weak π band

$$-\tau\Delta_1 + b\Delta_1^3 - \sum_j \xi_{1,j}^2 D_j^2 \Delta_1 - S_{12}\sum_{s=0}^{\infty}\left(f_s - \frac{\Delta_1}{s+1/2}\right) = 0, \tag{16a}$$

$$(s+1/2)f_s - \frac{2}{\pi^2}\xi_{2,z}^2 D_z^2 f_s = \Delta_1, \tag{16b}$$

$$j_j \approx 4eN_1\xi_{1,j}^2 \mathrm{Im}[\Delta_1^* D_j \Delta_1] + \delta_{j,z}\frac{8e}{\pi^2} N_1 S_{12}\xi_{2,z}^2 \sum_{s=0}^{\infty} \mathrm{Im}[f_s^* D_z f_s]. \tag{16c}$$

We explore now some consequences of these equations. To define an effective coherence length, we consider the response of the order parameter to the weak z-dependent variation of T_c, $\tau \to \tau(z) = \tau + \delta\tau(z)$. In linear approximation with respect to $\delta\tau(z)$ Eqs. (16a) and (16b) can be solved by Fourier transform yielding $\Delta_1 = \Delta_1^{(0)} + \delta\Delta_1(z)$

$$\delta\Delta_1(z) = \int G(z-z')\delta\tau(z')dz',$$

$$G(z) = \int \frac{dk}{2\pi}\frac{\exp(ikz)}{2\tau + \xi_{1,z}^2 k^2 + S_{12}g[(2/\pi^2)\xi_{2,z}^2 k^2]},$$

where $g(u) \equiv \psi(1/2+u) - \psi(1/2)$ and $\psi(u)$ is the digamma function. In contrast to the GL model, the decay of the perturbation $\delta\Delta_1(z)$ is not exponential. Using the last equation, one can introduce the effective coherence length ξ_z, which determines the scale of spatial variations of the order parameter in the z direction,

$$\xi_{1,z}^2/\xi_z^2 + S_{12}g[(2/\pi^2)\xi_{2,z}^2/\xi_z^2] = \tau. \tag{17}$$

The dependence $\xi_z(T)$ computed from this equation using parameters $S_{12} = 0.034$ [12] and $\xi_{2,z}^2 = 300\xi_{1,z}^2$ is shown in Fig. 1.

Consider the relation between the supercurrent j_z and supermomentum $p_z = \nabla_z\phi - (2\pi/\Phi_0)A_z$, which determines the c axis London length and depairing current. From Eqs. (16a) and (16b) we obtain

$$j_z(p_z) = 4eN_1\Delta_1^2(p_z)p_z \times \left\{\xi_{1,z}^2 + \sum_{s=0}^{\infty}\frac{(2/\pi^2)S_{12}\xi_{2,z}^2}{[s+1/2+(2/\pi^2)(\xi_{2,z}p_z)^2]^2}\right\},$$

$$\Delta_1^2(p_z) = \{\tau - \xi_{1,z}^2 p_z^2 - S_{12}g[(2/\pi^2)\xi_{2,z}^2 p_z^2]\}/b. \tag{18}$$

In the linear regime $j_z \approx (4e\tau N_1/b)(\xi_{1,z}^2 + S_{12}\xi_{2,z}^2)p_z$. This means that in the whole range $(T_c - T)/T_c \ll 1$ the z component of the London length is given by the GL formula (11). In conventional superconductors the dependence $j_z(p_z)$ is nonmonotonic and its maximum gives the well-known GL result for depairing current, $j_{dp} = c\Phi_0/(12\sqrt{3}\pi^2\lambda^2\xi) \propto \tau^{3/2}$ for $\tau \to 0$ [2]. In our case the situation is different. The amplitude of the order parameter is suppressed at $p_z \sim 1/\xi_z(T)$. However, in the region $\xi_z(T) \ll \xi_{2,z}$ the dependence $j_z(p_z)$ becomes nonlinear at much smaller p_z, $p_z \sim 1/\xi_{2,z}$. The shape of this dependence is determined by the parameter $S_r = S_{12}\xi_{2,z}^2/\xi_{1,z}^2$. The dependencies $j_z(p_z)$ for $S_r = 6$ and different temperatures are plotted in the left panel in Fig. 2. For large values of S_r the dependence $j_z(p_z)$ has *two maxima* within some temperature range, where first (second)

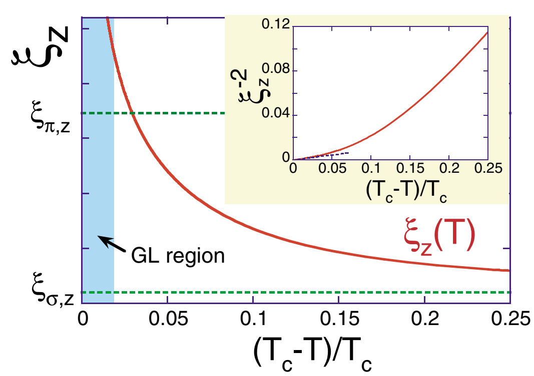

FIG. 1 (color online). Temperature dependence of the c axis coherence length, $\xi_z(T)$, computed from Eq. (17) with parameters $S_{12} = 0.034$ and $\xi_{2,z}^2 = 300\xi_{1,z}^2$. The marked GL region corresponds to condition $\xi_z(T) > \xi_{\pi,z} \equiv \xi_{2,z}$. The inset shows dependence $\xi_z^{-2}(T)$ with the dashed line showing the linear GL asymptotics at $T \to T_c$.

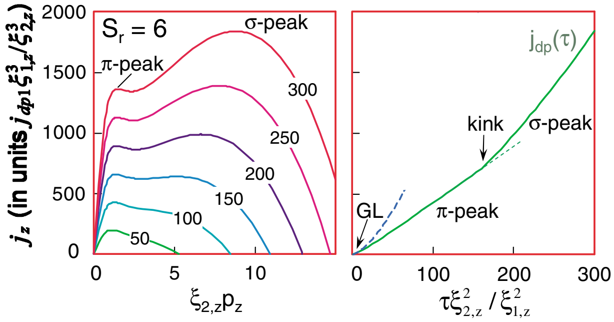

FIG. 2 (color online). Left panel: Dependencies $j_z(p_z)$ at different temperatures for $S_r = 6$. The curves are marked by the reduced temperatures $\tau\xi_{2,z}^2/\xi_{1,z}^2 = 50, \ldots, 300$. In the unit of the vertical axis $j_{dp1} = 4eN_1\xi_{1,z}/b$ is the depairing current scale for the σ band. Right panel: The temperature dependence of the depairing current for the same value of S_r. The dashed curve shows GL dependence.

maximum corresponds to the suppression of supercurrent in the π (σ) band. At low temperatures the depairing current j_{dp} is given by the second maximum and is determined mainly by the σ band. At a certain temperature near T_c global maximum switches to the first maximum (see Fig. 2). The temperature dependence of j_{dp} has a kink at this temperature (see the right panel in Fig. 2). For $S_r > 6$ the local maximum of $j_z(p_z)$ at $p_z \sim 1/\xi_{2,z}$ exists even in the limit $\xi_z(T) \ll \xi_{2,z}$.

As another example, we compute from Eqs. (16) the in-plane upper critical field near T_c, $H_{c2,a}(T)$. Experiment [7] shows strong upward curvature of $H_{c2,a}(T)$, leading to the temperature-dependent anisotropy factor. Microscopic calculations reproduce this feature, in both clean [8] and dirty [10] cases, but require rather heavy numerical computations. Our model allows one to trace the origin of the upward curvature in a simple way. Selecting the gauge $A_z = Hx$ and introducing reduced variables $h = H/H_{c2}^{(1)}$ with $H_{c2}^{(1)} \equiv \Phi_0/(2\pi\xi_{1,x}\xi_{1,z})$, $x \to \sqrt{h}x/\xi_{1,x}$, $r_z = \mathcal{D}_{2,z}/\mathcal{D}_{1,z}$, we write the linear equation for determination of the upper critical field, $h = H_{c2}/H_{c2}^{(1)}$, as

$$-\frac{S_{12}}{h}\sum_{s=0}^{\infty}\left(\frac{\Delta_1}{s+1/2} - f_s\right) - \nabla_x^2\Delta_1 + x^2\Delta_1 = \frac{\tau}{h}\Delta_1, \quad (19a)$$

$$(s+1/2)f_s + \frac{2}{\pi^2}r_z h x^2 f_s = \Delta_1. \quad (19b)$$

Excluding f_s, we obtain the Schrödinger equation for Δ_1 with nonparabolic potential

$$-\nabla_x^2\Delta_1 + \left(x^2 + \frac{S_{12}}{h}g\left[\frac{2r_z h x^2}{\pi^2}\right]\right)\Delta_1 = \frac{\tau}{h}\Delta_1. \quad (20)$$

Only in the limit $h \ll \sqrt{1+S_{12}r_z}/r_z \ll 1$ this equation reduces to the usual oscillator equation. In this limit, using expansion $g(u) \approx (\pi^2/2)u$, we reproduce the GL result, $h_{c2} = \tau/\sqrt{1+S_{12}r_z}$. The inequality $h_{c2} \ll \sqrt{1+S_{12}r_z}/r_z$ reproduces criterion (13) for the validity of the GL theory. In the opposite limit, $\sqrt{1+S_{12}r_z}/r_z \ll h \ll 1$, one can use the asymptotics $g(u) \approx \ln(4u) + \gamma_E$ for $u \gg 1$, with $\gamma_E \approx 0.577$ being the Euler constant, and obtain

$$-\nabla_x^2\Delta_1 + \left[x^2 + \frac{S_{12}}{h}\ln(x^2)\right]\Delta_1 = \alpha(h)\Delta_1,$$

$$\tau = \alpha(h)h + S_{12}\left(\ln\left[\frac{8hr_z}{\pi^2}\right] + \gamma_E\right).$$

This gives the following equation for the upper critical field:

$$h_{c2} + S_{12}\ln[Ch_{c2}r_z] = \tau,$$

with $C \sim 1$ $\{C \approx (8/\pi^2)\exp[\langle\ln(x^2)\rangle + \gamma_E] = 2/\pi^2$ for $h \gg S_{12}\}$. In this limit the π band gives only small logarithmic correction to the upper critical field. As we can see, the upper critical field has a strong upward curvature in a narrow region near T_c: the slope $dh_{c2}/d\tau$ changes from $1/\sqrt{1+S_{12}r_z}$ to 1 near $\tau = S_{12} + 1/r_z$, in agreement with microscopic calculations and experiment.

In conclusion, we demonstrated that the properties of magnesium diboride are not described by the anisotropic GL theory. We derived a simple model, which replaces this theory in the vicinity of T_c, and explored some consequences of this model.

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