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On the Role of Chemical Potential in Determining the Temperature Dependent Critical Magnetic Field and the Penetration Depth of Superconductors

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Abstract

Dealing with both elemental and high-T_c superconductors (SCs) - Sn, Nb and Pb belonging to the former category, and MgB_2 and different samples of YBCO to the latter - we show that the difference in the values of their critical magnetic field $H_{c1,c2}$ and the penetration depth $\lambda_L(0)$ is, remarkably, attributable predominantly to the difference in the values of a single parameter, viz., the chemical potential (μ) close to their critical temperatures (T_cs). Based directly on the dynamics of pairing in a magnetic field and the corresponding number equation, our approach relates $H_{c1,c2}$ of an SC with the following set of its properties: $S_1 = \{\mu, T_c$, *Debye temperature*, *effective mass of the electron*, *magnetic interaction parameter*, *Landau index*$\}$. Hence, it provides an alternative to the approach followed by Talantsev [Mod. Phys. Lett. B **33**, 1950195 (2019)] who has shown by ingeniously combining the results of various well-established theories that H_{c2} of an SC can be calculated via four different equations, each of which invokes two or more properties from its sample-specific set $S_2 = \{T_c$, *gap*, *coherence length*, $\lambda_L(0)$, *jump in sp. ht.*$\}$, which is radically different from S_1.

Keywords

Pairing and Number Equations Incorporating Temperature, Chemical Potential and Magnetic Field, Critical Magnetic Field, Penetration Depth, Sn, Nb, Pb, MgB_2, YBCO

1. Introduction

It is well known that the properties of a superconductor (SC) differ not only from one SC to another, but also from sample to sample of the same SC - depending on the sample geometry, size, nature of doping, manner of preparation, etc. Thus, for example, two samples of $YBa_2Cu_3O_7$ have been found to have the values of their critical temperature (T_c) and the upper critical magnetic field $H_{c2}^{c}(0)$ at temperature $T = 0$ when the applied field H is along the c-direction as given below [1].

$YBa_2Cu_3O_{6.5}$: $T_c = 62$ K, $H_{c2}^{c}(0) = 87\times10^4$ G

$YBa_2Cu_3O_{7-\delta}$ (with $\delta \approx$ near-optimal value of doping): $T_c = 92.4$ K,

$$H_{c2}^{c}(0) = 34\times10^4 \text{ G} \tag{1}$$

Pertaining to a different pair of samples (with unspecified values of δ) of the same SC and direction of the applied field, the values of T_c and the London penetration depth $\lambda_L^{ab}(0)$ below provide another example [1].

$$\begin{aligned} &\text{Sample 1:}\quad T_c = 66 \text{ K},\quad \lambda_L^{ab}(0) = 260 \text{ nm} \\ &\text{Sample 2:}\quad T_c = 92 \text{ K},\quad \lambda_L^{ab}(0) = 89 \text{ nm} \end{aligned} \tag{2}$$

Employing the examples of both elemental SCs (Sn, Nb and Pb) and high-T_c SCs (MgB_2 and two samples of YBCO), it is the purpose of this paper to show that the difference in the above-noted properties of these SCs can be understood predominantly on the basis of the difference in the values of a single parameter that characterizes them. This parameter, remarkably, is μ_1, *i.e.*, the value of the chemical potential μ at t_1 ($\equiv T_1/T_c$) close to 1 (say, 0.9) and hence amenable to experimental verification. The ramifications/implications of this result will be discussed. Before we do so, however, we give below a brief account of some of the earlier approaches to calculating H_{c2} of an SC in order to highlight the difference between them and the approach followed in this paper.

The most widely employed approach for the calculation of H_{c2} (B_{c2} in the SI system of units) is due to Werthamer, Helfand and Hohenberg (WHH) [2], which is based on the electron spin and spin-orbit effects. The WHH equation is

$$\ln\left(\frac{T}{T_c(B=0)}\right) = \psi\left(\frac{1}{2}\right) - \psi\left(\frac{1}{2} + \frac{\hbar D B_{c2}(T)}{2\phi_0 kT}\right),$$

where ψ is the Euler's digamma function, D the diffusion constant for the normal electrons/holes in the conduction band, $\phi_0 = 2.07\times10^{-15}$ Wb the flux quantum and k the Boltzmann constant. An older equation for B_{c2} in the classical two-fluid Gorter-Casimir model [3] is

$$B_{c2}(t) = \frac{\phi_0}{2\pi\xi_0^2}\left(1-t^2\right),$$

where ξ_0 is the coherence length at $t = 0$. A variant of the above equation is the Jones-Hulm-Chandrasekhar model [4]

$$B_{c2}(t)=\frac{\phi_0}{2\pi\xi_0^2}\frac{1-t^2}{1+t^2}.$$

Finally, the following equation for B_{c2} given by Gor'kov [5] is also said to provide a good fit to the data over the entire range of temperature

$$B_{c2}(t)=B_c(t)\frac{\sqrt{2}}{1.77}\frac{\lambda_0}{\xi_0}\left(1.77-0.53t^2+0.07t^4\right),$$

where $B_c(t)$ is the thermodynamic critical field.

It is interesting to note that combining each of the models noted above with a mix of the other properties of the SC, e.g., its gap Δ and the jump in the specific heat, Talantsev [6] has recently derived four new equations for B_{c2} each of which leads to nearly as good a fit to the empirical data of compressed H_3S as the other. It is notable that all of these approaches including that of Talantsev determine B_{c2} *indirectly* via the effects it has on one or more properties of the SC such as ξ_0 and λ_0. In contrast with these, the approach followed in this paper determines H_{c2} *directly* via the dynamics of pairing, *i.e.*, by employing an H_{c2}-dependent pairing equation (PE) together with the corresponding number equation (NE). Below, we will return to a further discussion of Talantsev's work and draw attention to how our approach complements his approach.

The PE and the NE on which the present study is based are given in the next section. Both of these equations are μ-, T- and H-dependent. These are supplemented by the equation for $\lambda_L(0)$. Procedural details of the application of these equations to both elemental and high-T_c SCs are given in Section 3. The final section sums up our findings.

2. The Core Equations

2.1. The μ-, T- and H-Dependent Pairing Equation (PE)

The PE is obtained via a 4-d Bethe-Salpeter equation (BSE) the 4th dimension of which is employed to temperature-generalize it via the Matsubara prescription. Subjecting the resulting 3-d equation to the Landau quantization scheme further generalizes it to include an applied magnetic field leading to the quantization of the transverse components of momentum into Landau levels. Finally, the PE employed here is obtained from this 1-d equation by putting the binding energy/gap $\Delta = 0$, whence it gives the value of the critical magnetic field H_c at any T or, equivalently, T_c corresponding to any H. Derived in [7] and subjected to a correction [8], this equation is reproduced below from the latter reference where it was shown to provide the basis of a new microscopic approach for dealing with the T- and H-dependent critical current densities of SCs.

$$1-\lambda_m\int_{L_1(..)}^{L_2(..)}\frac{\mathrm{d}\xi}{\sqrt{1+\xi/\mu}}\sum_{n=0}^{N_{L1}(..)}\frac{\tanh\left[\frac{\xi}{2kT}+\frac{\hbar\Omega(H_c)}{2kT}(n+1/2)\right]}{\xi+\hbar\Omega(H_c)(n+1/2)}=0, \tag{3}$$

where

$$\lambda_m = \frac{eH_cV}{16\pi^2}\sqrt{\frac{2\eta m_e}{\mu}},\ \mu = \rho k\theta,\ L_1(..) = \frac{-k\theta}{3}(2\rho+1),\ L_2(..) = \frac{k\theta}{3}(-2\rho+1)$$

$$N_{L1}(..) = floor\left[\frac{2}{3}\frac{(\rho+1)k\theta}{\hbar\Omega(H_c)} - \frac{1}{2}\right],\ \Omega(H_c) = \Omega_0 H_c/\eta,\ \Omega_0 = 1.7588\ \mathrm{s}^{-1}\cdot\mathrm{G}^{-1}$$

The parameter λ_m is the magnetic interaction parameter corresponding to temperature T, applied field H and the chemical potential μ which has been parametrized in terms of the Debye temperature of the SC as $\rho k\theta$, where k is the Boltzmann constant and ρ a free parameter; - V ($V > 0$) is the usual BCS model interaction due to the ion-lattice and Coulomb repulsion between electrons and finally, m_e is the mass of an electron and η its enhancement factor.

2.2. The μ-, T- and H-Dependent Number Equation (NE)

Also reproduced from [8], the NE is:

$$N_s(...) = C_1(hH_c)^{3/2}\int_0^{\sqrt{L(..)}}\sum_{n=0}^{N_2(..)}F(...)\mathrm{d}z,\ (h \neq 0) \tag{4}$$

where

$$C_1 = 2.1213\times10^9,\ t = T/T_c,\ h = H/H_c,\ L(..) = \frac{1}{3}\frac{(\rho q+1)k\theta}{\hbar\Omega(h_c)}$$

$$N_2(..) = floor\left[\frac{2}{3}\frac{(\rho q+1)k\theta}{\hbar\Omega(h_c)} - \frac{1}{2}\right]$$

$$F(...) = \left[1 - \tanh\left\{\frac{\hbar\Omega(h)}{2ktT_c}\left(n + 1/2 + z^2 - \frac{q\rho k\theta}{\hbar\Omega(h)}\right)\right\}\right]$$

The PE and NE are supplemented by the equation for the London penetration depth

$$\lambda_L(0) = \sqrt{\frac{\varepsilon_0\eta m_e c^2}{N_s e^2}},\quad \text{(SI Units)} \tag{5}$$

where $\varepsilon_0 = 8.85\times10^{-12}$ F·m^{-1}, c is the velocity of light, e the electronic charge, and N_s is as given by (4).

3. Procedural Details

In the following

$$t_1 = T_1/T_c,\ h_{c1,c2}(t_1) = H_{c1,c2}(T_1)/H_{c1,c2}(0)$$
$$t_0 = T_0/T_c,\ h_{c1,c2}(t_0) = H_{c1,c2}(T_0)/H_{c1,c2}(0),$$

where $t_1 = 0.9$ and $t_0 = 0.1$ for reasons to be specified.

3.1. Elemental SCs

In order to show that the properties of an SC in an external field are determined predominantly by $\mu(t_1)$, we proceed as follows.

1) Solve (3) for any SC to obtain the value of λ_{m1} with the input of its empirically listed values of T_c, H_c, an *assumed* value of $\mu_1 = \rho k\theta$ (ρ a free parameter), $t_1 = 0.9$ and the relation

$$h_c(t) = H_c(t)/H_c = 1 - t^2, \tag{6}$$

which for the most part has been found to be sound empirically and leads to $h_{c1} = 0.19$. Employment of this relation has been necessitated because, in general, the value of h_{c1} at t_1 is not known. Note that the choice of $t_1 = 0.9$ does away with the need to specify the self-field, which would be needed for $t = 1$ because then $h_{c1} = 0$, whereas a non-zero value of the latter is required for the employment of (4).

2) After λ_{m1} is determined as noted in 1), solve (3) to determine the value of μ_0 corresponding to the values of $t_0 = 0.1$ and $h_{c0} = 0.99$ via (6). The reason for choosing $t = 0.1$ and not 0 is that the listed value of any parameter at $t = 0$ is *invariably* one that is extrapolated from a low value of t because no experiment has ever been performed exactly at $T = 0$. This will be further discussed below. Since μ_1 was parametrized as $\rho k\theta$, if we define $\mu_0 = q\mu_1$, then it means that we are now solving the equation for q by replacing ρ by $q\rho$ in the earlier equation that yielded the value of λ_{m1}. Of course, we also need the value of λ_{m0} in order to obtain the value of q, which is easily obtained from the expression for λ_m given below (3) by noting that

$$\frac{\lambda_{m0}}{\lambda_{m1}} = \frac{h_{c0}}{h_{c1}}\frac{1}{\sqrt{q}},$$

since $\mu_0 = q\mu_1$. For the sake of concreteness, we write below the equation from which q is calculated. In terms of the dimensionless variable $x = \xi/2ktT_c$, this equation is

$$1 - \lambda_{m1}\frac{h_{c0}}{h_{c1}}\frac{1}{\sqrt{q}}\int_{x_1(..)}^{x_2(..)}\sum_{n=0}^{N_{L0}(..)}\frac{\mathrm{d}x}{\sqrt{1+\dfrac{2t_0T_c}{q\rho\theta}x}}\frac{\tanh\left[x+(n+1/2)\dfrac{\hbar\Omega(h_{c0})}{2kt_0T_c}\right]}{\left[x+(n+1/2)\dfrac{\hbar\Omega(h_{c0})}{2kt_0T_c}\right]} = 0, \tag{7}$$

where

$$x_1(..) = \frac{-\theta}{6t_0T_c}(2\rho q+1),\ x_2(..) = \frac{\theta}{6t_0T_c}(-2\rho q+1)$$

$$N_{L0}(..) = floor\left[\frac{2}{3}\frac{k\theta}{\hbar\Omega(h_{c0})}(\rho q+1) - \frac{1}{2}\right].$$

3) For the remainder of our procedure, it is convenient to deal with a specific SC, say Nb, for which $\lambda_L(0) = 52$ nm [1]. With the values of θ, η, T_c and H_c given in **Table 1**, the choice of the free parameter $\rho = 10$ leads via (3) to $\lambda_{m1} = 1.212 \times 10^{-6}$ and thence to $q = 2.607$, $N_s = 2.81 \times 10^{28}$ m^{-3} and $\lambda_L(0) = 109.8$ nm via (4) and (5), respectively. Since the last of these values is more than twice its listed value, we now repeat the steps carried out for $\rho = 10$ by progressively increasing ρ. Thus, we find that $\rho = 30.7$ leads to $\lambda_L(0) = 51.96$ nm. The values of the other parameters corresponding to these are given in **Table 1**, which includes the final results for not only Sn and Pb, but also MgB_2 and YBCO.

Table 1. The empirical values for elemental SCs in column 1 are taken from Poole [1] and the values of η from Kittel [9], except for Nb for which it is taken from Ashcroft and Mermin [10]. The equations employed to obtain the values of various parameters are as follows: λ_{m1} and N_{L1} via (3); q, $\lambda_{m0}(t_0)$ and N_{L0} via (7) and N_s and $\lambda_L(t_0)$ via (4) and (5), respectively. For the values of the parameters pertaining to MgB_2 and YBCO in column 1, see (8) and (9), respectively. YBCO/Y and YBCO/Ba mean that the 1PEM is due to the Y- and Ba-ions, respectively.

SC θ, T_c(K) $\eta = m_e^*/m_e$ $H_{c1}(G)$ $\lambda_L(0)$ (nm)	ρ	$\mu_1 = \rho k\theta$ (eV)	λ_{m1}	N_{L1}	$q = \frac{\mu_0}{\mu_1}$	λ_{m0}	N_{L0}	$N_s(t_0)\times 10^{28}$ (m^{-3})	$\lambda_L(t_0)$ (nm)
Sn 195, 3.72 1.26 305 42	148	2.49	2.192×10^{-6}	3,134,994	1.975	8.125×10^{-6}	1,184,352	2.029	41.87
Pb 96, 7.2 1.97 800 39	249	2.06	9.075×10^{-6}	1,543,592	2.27	3.139×10^{-5}	670,971	3.675	38.9
Nb 276, 9.25 12 1580 52	30.7	0.730	1.074×10^{-6}	1,735,552	2.356	3.645×10^{-6}	770,501	12.55	51.96
MgB_2 1062, 39 3.1 2.5×10^4 140	2.32	0.212	2.331×10^{-5}	11,418	3.055	6.948×10^{-5}	5538	0.447	139.9
YBCO/Y 410, 92 3.0 112×10^4 89	6.77	0.239	4.427×10^{-3}	222	5.506	9.831×10^{-3}	210	1.070	88.89

Continued

YBCO/Ba 478 [8], 92 3.0 112×10^4 89	6.2	0.255	3.630×10^{-3}	240	5.139	8.343×10^{-3}	210	1.072	88.88
YBCO/Y 410, 66 3.0 91×10^4 260	1.264	0.045	4.245×10^{-3}	79	6.516	8.666×10^{-6}	62	0.125	260.0

3.2. MgB_2 and YBCO

The procedural details for dealing with these SCs are similar to those for the elemental SCs, except that in the BSE-based approach which leads to a generalization of the BCS equations (GBCSEs) via the employment of a superpropagator, explanation of the values of its T_c and multiple gaps requires invoking more than a 1-phonon exchange mechanism (1PEM) for the formation of Cooper pairs. This is in contrast to the situation for elemental SCs for which 1PEM suffices. Hence, the question is: Do we require, say, 2PEM to deal with the properties of a composite SC in a magnetic field? The answer to this question is: not necessarily, because for the SCs considered here, the magnetic interaction parameter, *i.e.*, λ_m in (3), due to the B-ions in MgB_2 (Mg plays a secondary role via the proximity effect), or due to the Y- or Ba-ions ions in YBCO, turns out to be considerably smaller (and well below the Bogoliubov upper limit of 0.5) than any of the non-magnetic interaction parameters that occur in the equations for their T_c and the gaps [11].

For MgB_2, we now need to resolve $\theta(MgB_2)$ = 815 K which is the mean of its values given in [12] into θ_B and θ_{Mg}. The basic idea here is due to Born and Karmann [13] [14] who had pointed out a long time ago that elastic waves in an anisotropic solid travel with different velocities in different directions and are hence characterized by different Debye frequencies or temperatures. Employing the double-pendulum model for the resolution of $\theta(MgB_2)$ into the θs of its constituents [15], we obtain [11] θ_B = 1062 K and θ_{Mg} =322 K (which we will not need). The basis for the value of each of the other properties of MgB_2 noted in column 1 of **Table 1** is as follows

$$T_c = 39\ \text{K}\ \ [12],\ \ \eta = 3.1\ \ [16]$$
$$H_{c2} = 2.5\times 10^4\ \text{G}\ \ (H \| c)\ \ [12],\ \ \lambda_L^{ab}(0) = 140\ \text{nm}\ \ [17] \tag{8}$$

When the 1PEM is considered to be due to the Y ions in YBCO, the values of the above parameters are:

$\theta_Y = \theta$(YBCO) = 410 K [1] (because the sub-lattice that contains the Y ions has no other constituent)

$$T_c = 92 \text{ K} \quad [1], \quad \eta = 3.0 \quad [18]$$
$$H_{c2} = 112 \times 10^4 \text{ G} \ (H \| c) \quad [19], \quad \lambda_L^{ab}(0) = 89 \text{ nm} \quad [1] \tag{9}$$

It is seen from Table 1 that when the 1PEM is considered to be due to the Y ions, $\lambda_L(t_0) \approx 89$ nm is obtained when $\mu_1 = 0.240$ eV and that nearly the same value for $\lambda_L(t_0)$ results when the IPEM is considered to be due to the Ba ions with $\mu_1 = 0.255$ eV.

3.3. Dealing With Two Samples of YBCO that Have Significantly Different Values of T_c and $\lambda_L(0)$

Of the samples the properties of which were noted in (2), we have already dealt in detail with Sample 2 that has $T_c = 92$ K and $\lambda_L^{ab}(0) = 89$ nm. We now deal with Sample 1 of the same SC which is characterized by $T_c = 66$ K and $\lambda_L^{ab}(0) = 260$ nm. H_{c2} of this sample may be estimated to be 91×10^4 G, since $H_{c2} = 87 \times 10^4$ G for the sample for which $T_c = 62$ K - vide (1). The last row in Table 1 gives the values of all the parameters corresponding to $\lambda_L^{ab}(0)$ of Sample 1.

4. Summing Up

It has been shown in this paper that one can choose for any SC, via the choice of ρ, any value of $\mu(t_1)$ from among a multitude of them and find a value of $\mu(t_0)$ corresponding to it which is consistent with the empirical value of $H_{c1,c2}(t_0)$ of the SC for t_0 close to 0. However, demanding that the so-obtained value of $H_{c1,c2}(t_0)$ should also lead to the empirical value of $\lambda_L(t_0)$ of the SC fixes μ_1 uniquely.

It is seen from Table 1 that the value of $\mu_0 = q\mu_1$ (which is ≈ Fermi energy, E_F) for MgB_2, or any sample of YBCO, is considerably smaller than its value for the elemental SCs. This is in accord with the general belief that high-T_c superconductivity is governed by low values of E_F; see, e.g., [20].

It is interesting to note that we have adopted in this paper a variant of a part of the template given by Dogan and Cohen [21] to deal with various properties of SCs where the route to the value of $\lambda_L(0)$ is provided by the following equations

$$\xi_0 = \sqrt{\frac{\phi_0}{2\pi H_{c2}(0)}} \tag{10}$$

$$v_F = \frac{\pi \Delta_0 \xi_0}{\hbar} \tag{11}$$

$$N_s(0) = \frac{1}{3\pi^2}\left(\frac{m_e^2 v_F^2}{\hbar^2}\right)^{3/2}, \tag{12}$$

followed by (5) for the calculation of $\lambda_L(0)$; ϕ_0 above denotes the magnetic flux quantum and Δ_0 and ξ_0 denote the gap and the coherence length, respectively. The application of the above equations to YBCO with $H_{c2}(0) = 112$ T, $\Delta_0 = 20$ meV leads to

$$\xi_0 = 1.71\ \text{nm},\ v_F = 1.64\times10^5\ \text{m/s},\ N_s = 9.54\times10^{25}\ \text{m}^{-3},\ \lambda_L(0) = 544\ \text{nm} \quad (13)$$

In the approach followed here on the other hand, m_e is replaced by ηm_e and the values of ξ_0 and Δ_0 are not required. Solution of (3) with the input of μ_1 then leads to the values of λ_{m0} and N_{L0}; that of (7) to the values of q, λ_{m0} and N_{L0}; $N_s(t_0)$ is obtained via (4) which is employed in lieu of (12) and, finally, $\lambda_L(t_0)$ is calculated via (5). It is notable that our approach leads to v_F(YBCO) = 3.9×10^5 m/s via $\mu_0 = q\mu_1$ and $v_F = \sqrt{2\mu_0/\eta m_e}\,c$ (μ_0 and m_e in units of electron-Volt) which is very close to the upper limit of the range (2.5×10^5 – 3.8×10^5 m/s) of the universal Fermi velocity of hydrides [22].

Since the lowest value of t adopted in this paper is 0.1, it is tacitly assumed that the values of the parameters on which λ_L depends change insignificantly on extrapolation from $t = 0.1$ to $t = 0$. This flattening of the $H_{c2}(t)$ vs. t plot for such values of t is in accord with the results obtained by Talantsev [6] for compressed H_3S by employing four different equations based on well-established theories. Each of these equations invoked two or more parameters from the sample-specific set of the SC comprising {T_c, *gap*, *coherence length*, $\lambda_L(0)$ and *jump in sp. ht.*} However, departures from this type of behavior, *i.e.*, a steep rise in the value of $H_{c2}(t)$ as $t \to 0$ which is reminiscent of the divergence of ξ as $t \to 1$, seem to have been empirically observed recently. For this reason, we believe that it is a good practice while quoting the value of any parameter to specify the lowest temperature at which it has been empirically determined (rather than reporting its extrapolated value) as has been done by Minkov, *et al.* [23] who have quoted the value of T as 10 K while reporting for compressed H_3S the values of ξ_0, λ_L, etc. For a further discussion of the possible departure of the value of $H_{c2}(t)$ from its value from, say $t = 0.1$, to lower values of t, we draw attention to [24] where a study of the $H_{c2}(t)$ of compressed H_3S and the issue of whether or not it satisfies the criterion of the Meissner effect was carried out by following the same approach as in this paper.

A significant result of this paper is that if we could find empirically for any SC the values of h_{c1}/h_{c2} at t_1 and the unique value of $\mu(t_1)$ that leads via $\mu(t_0)$ to the value of its $\lambda_L(t_0)$ by employing the equations that have been given, then we shall have a new, dynamics-based approach to calculate H_{c2} as an alternative to the existing approaches. We believe that this result is empirically verifiable. It is interesting to draw attention to yet another approach for the calculation of H_{c2} which is based on the thermodynamics of an SC in a magnetic field [25] and hence differs from all the other approaches including the one presented in this paper. It is worth noting that these different approaches ought to be viewed as complementing each other - rather than as competing approaches - because they shed light on different features of the same phenomenon. Finally, in so far as the practical applications are concerned, the study reported here suggests that by controlling the value of μ – which is a problem that belongs to the realm of chemical engineering - we could fabricate SCs that have bespoke properties.

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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