Condensation energy in the spin-fermion model for cuprates

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We compute the condensation energy in the spin-fermion model using Scalapino-White relation between the condensation energy and the change in the dynamical structure factor in the normal and the superconducting states. We show that for parameters relevant to cuprates, the extra low-frequency spectral weight associated with the resonance peak in the dynamical structure factor in a superconductor is not compensated up to energies \sim *J* which are much larger than the superconducting gap Δ . We argue that in this situation, the condensation energy is large and well accounts for the data for cuprates.

The understanding of the mechanism of superconductivity is an important step towards the general understanding of the physics of cuprates. It has been known from the studies of BCS superconductors, that the information about the pairing boson can be extracted from the measurements of the upper critical field. Specifically, the thermodynamic critical-field H_c is related to the condensation energy E_c by E_c $= V_0 H_c^2/(8 \pi)$, where V_0 is the volume of the unit cell. This condensation energy is the difference between the decrease of the potential energy associated with the feedback effect from superconductivity on the bosonic mode which is responsible for pairing, and the increase of the kinetic energy of electrons in a superconductor.¹ The calculations of E_c for phonon-mediated pairing yielded a good agreement with measured H_c and confirmed that phonons were responsible for pairing.

Recently, Scalapino and White² applied the same reasoning to cuprates. They argued that if the pairing is mediated by spin fluctuations, then the decrease of the potential energy in a superconductor is given by the difference in the dynamical structure factor $S(q,\Omega)$ between the normal and the superconducting states, integrated over frequency and momentum with the weighting factor (cos $q_x + \cos q_y$). This yields a relation^{2,3}

$$
\frac{H_c^2}{8\pi} = \frac{3}{2} \alpha J \int \frac{d^2 q d\Omega}{(2\pi)^3} \times (S_n(\mathbf{q}, \Omega) - S_{sc}(\mathbf{q}, \Omega))
$$

×(cos q_x + cos q_y), (1)

where α <1 is a numerical factor which accounts for the fact that the decrease of the potential energy in a superconductor is partly compensated by the increase of the kinetic energy.

Neutron-scattering experiments in bilayer YBCO and Bi2212 demonstrated^{4,5} that *S*(q , Ω) in a superconducting state possesses a resonance peak at momenta near **Q** $= (\pi,\pi)$ and at frequencies below 2 Δ where $\Delta \ll J$ is the maximum of the *d*-wave gap. The integrated intensity of the resonance peak (which is only observed in the odd channel of coupled spin fluctuations within a bilayer) yields the r.h.s. of Eq. (1) roughly consistent with the data on H_c .³

It is, however, not clear *a priori* to which extent the contribution from the resonance peak measures the decrease of the potential energy in a system. The point is that for large

Hubbard U (as in cuprates⁶), the double occupancy is energetically unfavorable, and the average value of the on-site spin *S* remains almost unchanged between the normal and the superconducting states. Since *S* is related to the dynamical structure factor by $\int d^2q d\Omega S(\mathbf{q},\Omega) = S(S+1)/3$, the total spectral weight in $S(q,\Omega)$ is nearly conserved, and the extra potential energy stored in the resonance peak below T_c has to be compensated by the depletion of the spectral weight in $S_{sc}(\mathbf{q},\Omega)$ at higher energies.

At large *U* the typical velocity of the spin excitations is comparable to J (see below). Hence, if the compensation comes from energies of order Δ , which are small compared to *J*, than typical $|\mathbf{q}-\mathbf{Q}|\ll 1$. For these **q**, the geometrical $\cos q_x + \cos q_y$ factor is nearly constant and only weakly affects the momentum integral in the r.h.s. of Eq. (1) . Obviously, in this situation, the r.h.s. of Eq. (1) is nearly zero, and the decrease in the potential energy is much smaller than one can extract by focusing solely on the the resonance peak. If, however, the compensation comes from energies comparable to *J*, than typical $|\mathbf{q}-\mathbf{Q}|$ are of order 1, and the momentum dependence of the geometrical factor cannot be neglected. In this situation, the gain in the potential energy is not substantially reduced by the sum-rule constraint and remains of the same order as the net contribution from the resonance peak.

In this paper, we compute the dynamical structure factor within the spin-fermion model for cuprates. We show that near optimal doping, when the pseudogap effects can be neglected, the compensation of the spectral weight stored in the resonance peak comes from high energies $\sim J$ or, equivalently, from momenta **q** far from **Q**. This result shows that the condensation energy is *not* in conflict with the sum rule, and justifies the use of the integrated area under the resonance peak as an estimate for the condensation energy in cuprates.

The point of departure for our consideration is the spinfermion model for cuprates. It describes low-energy fermions interacting with their own collective spin degrees of freedom.7,8 The fermionic spectral function has been discussed in detail in Ref. 8. Here we focus on the fully renormalized dynamical spin susceptibility $\chi(\mathbf{q},\Omega)$. It is related to the dynamical structure factor by $S(\mathbf{q},\Omega)=2\chi''(\mathbf{q},\Omega)/(1)$ $-e^{-\hbar\Omega/T}$). We argued earlier⁸ that both in the normal and the superconducting state, $\chi(\mathbf{q},\Omega)$ can be written as $\chi^{-1}(\mathbf{q}, \Omega) = \chi_0^{-1}(\mathbf{q}) - \Pi_{\mathbf{q}}(\Omega)$, where $\chi_0(\mathbf{q})$ is made pre-

dominantly out of fermions with energies comparable to bandwidth, and $\Pi_{\mathfrak{g}}(\Omega)$ is the extra universal (i.e., cutoff independent) contribution from low-energy fermions (see be $low).$

The form of $\chi_0(\mathbf{q})$ is the input for low-energy calculations. As before,⁸ we assume that $\chi_0(\mathbf{q})$ is peaked at or near **Q** and can be regularly expanded around the peak, i.e., $\chi_0(\mathbf{q}) = \chi_0 \xi^2/(1+(\mathbf{q}-\mathbf{Q})^2\xi^2)$. Here χ_0 and ξ are doping dependent overall factor and the magnetic correlation length, respectively. In principle, both χ_0 and ξ also depend on temperature and (in the superconducting state) on the pairing gap, Δ . However, simple estimates show that as $\chi_0(\mathbf{q})$ is dominated by fermions with energies comparable to the bandwidth *W*, the last two dependences are very weak and we neglect them.

The universal contribution to the dynamical susceptibility involves low-energy fermions and, as we will see, changes substantially between the normal and the superconducting states. Physically, the existence of this universal contribution to $\chi(\mathbf{q},\Omega)$ is related to the fact that for a Fermi surface with hot spots (as in cuprates), a low-energy spin excitation can decay into a particle-hole pair, and the energy conservation requires that both fermions in the pair remain near the Fermi surface. Near $q = Q$, one can neglect the q dependence in Π [it yields only a small correction to already existing dispersion in $\chi_0(\mathbf{q})$ and restrict with $\Pi_{\mathbf{Q}}(\Omega) = \Pi_{\Omega}$. The full susceptibility then has the form

$$
\chi(\mathbf{q}, \Omega) = \frac{\chi_0 \xi^2}{1 + (\mathbf{q} - \mathbf{Q})^2 \xi^2 - \Pi_\Omega}.
$$
 (2)

We absorbed $\chi_0 \xi^2$ into the redefinition of Π_{Ω} .

We discuss the computations of Π_{Ω} below but first consider what we actually need to compute. Our goal is to check how the extra spectral weight in local $S_{sc}(\Omega)$ is redistributed compared to the normal state. For this purpose, it is sufficient to compute the integral in Eq. (1) without the geometrical $\cos q_x + \cos q_y$ factor and check at which scales the sum rule is recovered.

Without $\cos q_x + \cos q_y$, the momentum integration in the r.h.s. in Eq. (1) can be performed exactly, and at $T\rightarrow 0$, we obtain

$$
I = \int \frac{d^2 q d\Omega}{(2\pi)^3} \left(S_{sc}(\mathbf{q}, \Omega) - S_n(\mathbf{q}, \Omega) \right)
$$

$$
= \frac{\chi_0}{4\pi^2} \int_0^\infty d\Omega \, \Delta S(\Omega), \tag{3}
$$

where $\Delta S(\Omega) = S_n(\Omega) - S_{sc}(\Omega)$, $S(\Omega) = \arctan((1$ $-\text{Re }\Pi_{\Omega}$)/Im Π_{Ω}), and S_n and S_{sc} are the values of $S(\Omega)$ in the normal and the superconducting states.

We now obtain Π_{Ω} . Diagrammatically, it is given by a sum of fully renormalized particle-hole bubbles made of normal and anomalous Green's functions. Expected universality of Π_{Ω} implies that this contribution is obtained by linearizing fermionic dispersion near hot spots. It also implies that the computation of Π_{Ω} has to be done self-consistently with the computation of the low-energy fermionic self-energy.

FIG. 1. The results for $\Delta S(\Omega) = S_n(\Omega) - S_{sc}(\Omega)$ from Eq. (3), obtained by the soluton of the full set of Eliashberg equations (Ref. 11). The frequency integral of $_\Delta S(\Omega)$ yields the condensation energy. The data sets are for (a) $2\Delta/\omega_{sf}$ 0.1, and (b) $2\Delta/\omega_{sf}$ 0.2, which corresponds to optimally doped YBCO. The frequency is measured in units of Δ . In the top figure, the resonance spin frequency Ω_{res} is indistinguishable from 2Δ . The arrows indicate the behavior which we obtained analytically for frequency independent anomalous vertex F (see text). Observe that in both cases $\int d\Omega_{\Delta} S(\Omega)$ is confined to frequencies which are substantially larger than 2Δ .

We make two approximations in computing Π_{Ω} . First, we assume that vertex corrections can be neglected, i.e., Eliashberg theory is valid. We have checked in the one-loop renormalization-group method (RG) formalism¹⁰ that vertex corrections slightly change the powers of frequency but do not modify any of the conclusions below. Second, for our analytic consideration, we approximate the anomalous pairing vertex $F(\omega)$ by a frequency independent constant *F* which we consider as an input parameter. The full analysis indeed requires one to solve a set of three coupled Eliashberg-type equations for the fermionic self-energy $\Sigma(\omega)$, anomalous pairing vertex $F(\omega)$, and Π_{Ω} (Ref. 11). We, however, also present in Fig. 1 the results of the full numerical solution of the Eliashberg set. We will see that analytical and numerical results fully agree with each other.

For $F(\omega) \approx F$, the coupled equations for Π_{Ω} and $\Sigma(\omega)$ related to the fermionic propagator by $G^{-1}(k,\omega) = \sum(\omega)$ $-v_F(k-k_F)$ have been derived in Ref. 8 and at $T=0$ have the form:

$$
\Sigma_{\omega} = \omega + \frac{\lambda}{2\pi} \int \frac{\Sigma_{\omega+\Omega}}{q_x^2 + \Sigma_{\omega+\Omega}^2 - F^2} \frac{d\Omega dq_x}{\sqrt{q_x^2 + 1 - \Pi_{\Omega}}} \tag{4}
$$

$$
\Pi_{\Omega} = \frac{i}{2} \int \frac{d\omega}{\omega_{sf}} \left(\frac{\Sigma_{\Omega - \omega} \Sigma_{\omega} + F^2}{\sqrt{\Sigma_{\Omega - \omega}^2 - F^2} \sqrt{\Sigma_{\omega}^2 - F^2}} + 1 \right). \tag{5}
$$

Here $\lambda = 3\bar{g}/(4\pi v_F \xi^{-1})$ is a dimensionless parameter which governs the strength of the spin-fermion coupling (we use the same notations as in Ref. 8: \overline{g} is the effective spinfermion coupling, and v_F is the Fermi velocity at a hot spot). In these notations, $\omega_{sf} = (3/16)v_F \xi^{-1}/\lambda$. By all experimental accounts, at and below optimal doping $\lambda \ge 1$, i.e., the model falls into the strong coupling regime. δ

In the normal state, the solution of Eqs. (4) and (5) is straightforward.⁸ For any coupling strength Π_{Ω} is linear in $\Omega: \Pi_{\Omega} = i |\Omega|/\omega_{sf}$. Hence, $S_n(\Omega) = \arctan(\omega_{sf}/|\Omega|)$. The fermionic self-energy has a Fermi-liquid form $\Sigma(\omega) = \lambda(\omega)$ $+i\omega|\omega|/(4\omega_{sf})$ at energies smaller than ω_{sf} , and at larger frequencies crosses over into a non-Fermi liquid, quantumcritical regime $\Sigma(\omega) \propto \exp(i\pi/4) \omega \sqrt{\frac{2}{g}}/|\omega|$. The quantumcritical behavior holds up to a frequency $\overline{\omega}$ which is independent on ξ and is of order $\min(\overline{g}, (v_F k_F)^2/\overline{g})$. Observe that at strong coupling, the crossover frequency ω_{sf} is parametrically smaller than $\overline{\omega}$, and hence the quantum-critical region is rather wide.

Consider now the superconducting state. A simple experimentation shows that the solution of Eqs. (4) and (5) depends on the ratio between ω_{sf} and twice the actual superconducting gap Δ , which is the solution of $\Sigma(\Delta)=F$. If $2\Delta \ll \omega_{sf}$, then at typical energies relevant to superconductivity, the system behaves as a renormalized Fermi liquid $(\Sigma(\omega))$ $\approx \lambda \omega$). In the opposite limit, $\omega_{sf} \leq 2\Delta$, fermions with ω $\sim \Delta$ display in the normal state the quantum-critical $\sqrt{\omega}$ behavior.

Below we consider separately both limiting cases ω_{sf} $\leq 2\Delta$ and $\omega_{\text{sf}} \geq 2\Delta$ where analytical treatment is possible, and we can identify all relevant scales. We show that in both limits the compensation of the spectral weight comes from frequencies which are parametrically larger than Δ . On the other hand, only at $\omega_{sf} \leq 2\Delta$, the typical momenta are not small, and the condensation energy is of order of the net contribution from the resonance peak, which by itself is sharp only if ω_{sf} is small compared to 2Δ .

We start with $\omega_{\rm sf} \geq 2\Delta$. Here the solution of $\Sigma(\Delta) = F$ falls into the Fermi-liquid regime, and hence the measured gap $\Delta = F/\lambda$. Using earlier results,⁹ we find that Im $\Pi_{\Omega} = 0$ for Ω <2 Δ and undergoes a finite jump to $\pi\Delta/\omega_{sf}$ at Ω = 2Δ . Due to the jump, Re Π_{Ω} logarithmically diverges at 2Δ , and this causes the resonance at $\Omega_{res} = 2\Delta(1)$ $- O(e^{-\omega_{sf}/2\Delta})$) where 1-Re Π_{Ω} changes sign. One can easily make sure that as Ω_{res} is exponentially close to 2Δ , the total spectral weight of the resonance peak is also exponentially small in $2\Delta/\omega_{sf}$.

Above 2 Δ , the analytical form for Π_{Ω} can be obtained in the limit of $\Omega \gg 2\Delta$. We found Re $\Pi_{Q}(\Omega) \approx \pi \Delta^2/(\Omega \omega_{sf})$ and Im $\Pi_{Q}(\Omega) = (\Omega/\omega_{sf}) + (2\Delta^2/(\Omega \omega_{sf}))\log(\Omega/\Delta)$. Substituting these results into Eq. (3) we find after a simple algebra that below 2Δ , $\Delta S(\Omega)$ is negative except for a tiny range between Ω_{res} and 2Δ , while above 2Δ , $\Delta S(\Omega)$ is positive and scales as $\Delta S(\Omega) \propto (1/\Omega) \log \Omega / \Delta$ for $\Omega \le \omega_{sf}$ and as $\Delta S(\Omega) \propto (1/\Omega)^3$ for $\Omega > \omega_{sf}$.

Splitting the integral in Eq. (3) in two parts, $I = I_1 + I_2$, where the first is the integral over frequencies up to twice the measured gap and the second is the integral over larger frequencies, and performing integration we obtain with the logarithmical accuracy

$$
I_1 \approx \frac{\chi_0}{4\pi^2} \left(\pi (2\Delta - \Omega_{res}) - \frac{2\Delta^2}{\omega_{sf}} \right) \approx -\frac{\chi_0}{2\pi^2} \frac{\Delta^2}{\omega_{sf}}
$$

$$
I_2 \approx \frac{\chi_0}{2\pi^2} \frac{\Delta^2}{\omega_{sf}} \int_{-\Delta}^{-\omega_{sf}} \frac{d\Omega}{\Omega} \log \frac{\Omega}{\Delta} \approx \frac{\chi_0}{4\pi^2} \frac{\Delta^2}{\omega_{sf}} \log^2 \frac{\omega_{sf}}{\Delta}.
$$
(6)

We see that the contribution from low frequencies is negative; the vanishing of Im Π_{Ω} below 2 Δ overshadows the extra contribution from the resonance peak. The total $I = I_1$ $+I_2$ is still positive due to contribution from frequencies above 2Δ . However, although typical frequencies in I_2 are much larger than Δ , still I_2 converges at $\omega > \omega_{sf}$. At ω $\sim \omega_{\text{sf}}$, $\Pi_{\Omega} = O(1)$, and hence typical $|\mathbf{q} - \mathbf{Q}|$ are of the order of inverse correlation length [see Eq. (2)]. For these **q**, the geometrical factor cos $q_x + \cos q_y$ is nearly a constant, i.e., there is almost no distinction between the condensation energy and the difference between $\int d^2q d\Omega S(\mathbf{q},\Omega)$ in the normal and the superconducting state. Alternatively speaking, at $2\Delta \ll \omega_{sf}$, the decrease of the potential energy in a superconductor is unrelated to the emergence of the (weak) resonance peak in the spin channel. A nonzero value of the condensation energy just reflects the fact that in the absence of no double occupancy constraint, the average on-site spin in the *d* wave superconducting state is smaller than in the normal state.

The analytical results are fully consistent with the full numerical solution of the Eliashberg set, 11 which we present in Fig. 1(a). Integrating $\Delta S(\Omega)$ from Fig. 1(a), we obtained $I_1 = -0.03$ ($\chi_0 \Delta/4\pi$) and $I_2 = 0.11$ ($\chi_0 \Delta/4\pi$).

Consider now the opposite limit of $\omega_{sf} \ll 2\Delta$. Here fermions with $\omega \sim \Delta$ display in the normal state the quantumcritical $\sqrt{\omega}$ behavior. Accordingly, the measured gap is now $\Delta \sim F^2/\overline{g}$. Analyzing the set Eqs. (4) and (5) using the spectral representations, we find that still Im $\Pi_{\Omega} = 0$ below 2Δ , but now the resonance condition Re $\Pi_{\Omega} = 1$ is satisfied at a small frequency $\Omega_{res} \sim (\Delta \omega_{sf})^{1/2} \ll \Delta$. This solution is unrelated to the jump in Im Π_{Ω} at 2 Δ , and is due to the fact that at small frequencies, Re $\Pi_{\Omega} \sim \Omega^2/(\Delta \omega_{sf})$, i.e., spin collective excitations in a superconductor behave as propagating magnons at frequencies well below 2Δ . As a result, $S(Q,\Omega)$ should have a sharp, almost δ functional peak at Ω_{res} .

At $\Omega \ge \Delta$ we found from Eqs. (4) and (5) that Im Π_{Ω} approaches the normal-state form $\left|\Omega\right|/\omega_{sf}$, but Re Π_{Ω} saturates at Re $\Pi_{\Omega} = \pi \beta \Delta/(2\omega_{sf})$ where $\beta = (1 + \pi^{-1} \log 4)$, and preserves this value as long as the fermionic propagator has a non-Fermi liquid, $\sqrt{\omega}$ form, i.e., up to $\omega \sim \overline{\omega}$.

Substituting the results for Π_{Ω} into Eq. (3) we find that $\Delta S(\Omega)$ is positive starting already from $\Omega = \Omega_{res} < 2\Delta$. Moreover, the saturation of Re Π_{Ω} above 2 Δ gives rise to a $1/\Omega$ behavior of $\Delta S(\Omega)$ which in turn gives rise to a logarithmical divergence of I_2 . Evaluating the integral in Eq. (3) with the logarithmical accuracy we obtain

$$
I_1 = \frac{\chi_0}{4\pi} (\Delta - \Omega_{res})
$$

$$
I_2 = \frac{\chi_0}{8\pi} \Delta \beta \int_{-\Delta}^{\overline{\omega}} \frac{d\Omega}{\Omega} = \frac{\chi_0}{8\pi} \Delta \beta \log \frac{\overline{\omega}}{\Delta}.
$$
(7)

We see that for $\Delta > \Omega_{res}$, I_1 is positive, i.e., at strong coupling, the appearance of the resonance peak below T_c gives rise to an extra integrated spectral weight below 2Δ and hence yields a positive contribution to the condensation energy. As we discussed before, this extra spectral weight should be compensated by a depletion of the spectral weight at higher frequencies. We see, however, that due to nonFermi-liquid behavior of the fermionic propagator above 2Δ , this depletion does not occur up to frequencies $\Omega \sim \overline{\omega}$. Moreover, the positive contribution to the condensation energy from frequencies above 2Δ is larger than I_1 .

Consider next which momenta chiefly contribute to the r.h.s. of Eq. (3). It follows from Eq. (2) that typical $|{\bf q}-{\bf Q}|$ are of order $(\bar{\omega}/(\omega_{sf} \xi^2))^{1/2}$. For $\bar{g} \gg v_F k_F$, which in the Hubbard-model language implies $U \ge t$, $\overline{\omega}$ is of order $(v_F k_F)^2 / \bar{g} \sim J$ and hence typical $|\mathbf{q} - \mathbf{Q}|$ are $O(k_F)$, i.e., they are comparable to inverse lattice spacing. In other words, the depletion of the spectral weight is confined to momenta which are far away from **Q**. For these momenta, the geometrical cos $q_x + \cos q_y$ factor in Eq. (1) cannot be approximated by a constant and therefore *the condensation energy is not substantially affected by the sum rule and remains of the same order as the net contribution from the resonance peak*. This is the central result of the paper.

The results of the numerical solution of the Eliashberg set for $2\Delta > \omega_{sf}$ are shown in Fig. 1(b). They clearly indicate that $_{\Delta}S(\omega)$ jumps at $\omega = \Omega_{res} < 2\Delta$, and slowly decreases at larger frequencies. For comparison with optimally doped YBCO and Bi2212, we present the results for $\Delta \sim \omega_{\rm sf}$ [experimentally, $\Delta \sim 25$ meV in optimally doped YBCO (Ref. 12), and \sim 35 meV in Bi2212 (Ref. 13), while $\omega_{sf} \sim 10-30$ meV (Ref. 7)]. We checked that for larger Δ/ω_{sf} , which correspond to underdoped cuprates, the behavior of ΔS is similar to that in Fig. $1(b)$.

Evaluating I_1 and I_2 numerically, we obtained $I_1=0.05$ $(\chi_0\Delta/4\pi)$ and $I_2=0.21$ ($\chi_0\Delta/4\pi$). The relative smallness of

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*I*₁ is indeed related to the fact that for chosen $2\Delta/\omega_{sf}$, Ω_{res} is comparable to Δ . For larger Δ/ω_{sf} , I_1 increases while I_2 does not change much.

Experimentally, in YBCO the frequency integral of the resonance peak $\int d\omega S(Q,\omega) = 0.52$ (Refs. 3 and 4). Using our form of *S*(Q , ω), we obtain $\chi_0 \approx 0.52a^2/(\pi \xi^2 \omega_{res})$ (Ref. 4), where *a* is Cu-Cu distance. Using ω_{res} ~ 40 meV (Ref. 5), $\xi \sim 1.5-2a$ (Ref. 7), we obtain $E_c \sim 6JI \approx 0.005J \sim 8-14$ K which agrees with $E_c \sim 3 - 12$ K extracted from specific-heat measurements.14

To summarize, in this paper we considered the condensation energy within the spin-fermion model for cuprates. At strong coupling, this model predicts that in a superconducting state, $S(Q,\Omega)$ possesses a sharp resonance peak below twice the maximum of the measured *d*-wave gap. We demonstrated that the appearance of this peak does not cause the depletion of the spectral weight in local $S(\omega)$ up to frequencies of order *J*. We computed the condensation energy E_c using Scalapino-White relation between E_c and $S(\mathbf{q},\Omega)$, and found that due to the absence of depletion in $S(\Omega)$ at low energies, the spin sum rule does not reduce the condensation energy. This disagrees with the assertion in Ref. 3 that large condensation energy cannot be obtained in the spin-fermion model. Moreover, we found that the contribution to E_c comes not only from the resonance peak but also from a wide range of frequencies up to *J*.

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