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Flux quantization and superfluid weight in doped antiferromagnets

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Abstract. Doped antiferromagnets, described by a t - t' - J model and a suitable $1/N$ expansion, exhibit a metallic phase-modulated antiferromagnetic ground state close to half-filling. Here we demonstrate that the energy of the latter state is an even periodic function of the external magnetic flux threading the square lattice in an Aharonov–Bohm geometry. The period is equal to the flux quantum $\Phi_0 = 2\pi\hbar c/q$ entering the Peierls phase factor of the hopping matrix elements. Thus flux quantization and a concomitant finite value of superfluid weight D_s occur along with metallic antiferromagnetism. We argue that in the context of the present *effective* model, whereby carriers are treated as hard-core bosons, the charge q in the associated flux quantum might be set equal to $2e$. Finally, the superconducting transition temperature T_c is related to D_s linearly, in accordance to the generic Kosterlitz–Thouless type of transition in a two-dimensional system, signalling the coherence of the phase fluctuations of the condensate. The calculated dependence of T_c on hole concentration is qualitatively similar to that observed in the high-temperature superconducting cuprates.

1. Introduction

During the last few years there has been some evidence that mobile holes in doped antiferromagnets, such as the high- T_c superconducting copper oxide layers [1], behave much like hard-core bosons. This transmutation of statistics, from bare fermionic holes to bosonic vacancy quasiparticles, should be understood as an ‘emergent phenomenon’ due to the reduced dimensionality and the presence of a strongly correlated spin background. In the context of the simple fermionic t - J model, proposed by Anderson [2] to describe such systems, the aforementioned evidence comes from exact-diagonalization studies of the ground-state energy and the static hole–hole correlation function on small clusters [3–5]. Indeed, the possibility of a hard-core boson behaviour of the charged vacancies in doped antiferromagnets, opening the way to Bose–Einstein condensation and the appearance of superconductivity, was suggested by many authors [6,7] in the early days of high- T_c superconductivity research. Thouless [7], in particular, argued that due to topological constraints, a vacancy in a two-dimensional torus lattice threaded by an external magnetic flux must be transported twice around the ring in order to recover its original configuration. Hence flux quantization with an effective charge $q = 2e$ may result from this period-doubling of the charge e bosons.

In all the aforementioned works, the lack of an effective model for doped antiferromagnets expressed in terms of hard-core bosons has prevented the systematic study of their flux quantization properties in conjunction with the optical and magnetic ones. Such

a model, however, has been postulated from the outset by Psaltakis and Papanicolaou [8] and consists of a $t-t'-J$ Hamiltonian and a suitable $1/N$ expansion that provide a reasonably simple many-body calculational framework for the study of the relevant issues. When leading quantum-fluctuation effects are taken into account in the context of this model, the generic experimental features of the optical conductivity, the Drude weight and the total optical weight in the cuprates are qualitatively reproduced. In particular, our theory [9, 10] accounts aptly for the experimentally observed 0.5 eV peak of the midinfrared band [11–13] and the mass enhancement factor approximately equal to 2 [12]. Furthermore, it predicts a finite limiting value for the optical conductivity $\sigma(\omega \rightarrow 0)$, at finite hole doping, consistent with the residual far-infrared conductivity observed in the $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ family of cuprates [14]. Our results are also found to be consistent with relevant exact-diagonalization data [15].

In view of the quoted evidence from optical experiments in favour of our effective model, we undertake in the present paper a systematic study of its flux quantization properties in order to provide a more complete assessment of the main electromagnetic responses. Our study includes results for the superfluid weight D_s and the associated superconducting transition temperature T_c . In particular, our explicit numerical estimates for the doping dependence of T_c , including leading quantum-fluctuation effects, are found to reproduce qualitatively the observed trends in the cuprates [16, 17].

2. Effective model

Our effective model is described by a $t-t'-J$ Hamiltonian expressed in terms of Hubbard operators $\chi^{ab} = |a\rangle\langle b|$ as

$$H = - \sum_{i,j} t_{ij} \chi_i^{0\mu} \chi_j^{\mu 0} + \frac{1}{2} J \sum_{\langle i,j \rangle} (\chi_i^{\mu\nu} \chi_j^{\nu\mu} - \chi_i^{\mu\mu} \chi_j^{\nu\nu}) \quad (1)$$

where the index 0 corresponds to a hole, the Greek indices μ, ν, \dots assume two distinct values, for a spin-up and a spin-down electron, and the summation convention is invoked. Here J is the antiferromagnetic spin-exchange interaction between nearest-neighbour sites $\langle i, j \rangle$ on a square lattice endorsed with periodic boundary conditions and a total number of sites $\Lambda = \Lambda_x \times \Lambda_y$, where $\Lambda_x = \Lambda_y$. For the hopping matrix elements t_{ij} we assume

$$t_{ij} = \begin{cases} t & \text{if } i, j \text{ are nearest neighbours} \\ -t' & \text{if } i, j \text{ are next nearest neighbours} \\ 0 & \text{otherwise.} \end{cases} \quad (2)$$

The conventions in (2) incorporate opposite signs for t and t' as dictated by quantum-chemistry calculations [18, 19] for Cu–O clusters and fits of the shape of the Fermi surface observed by angle-resolved photoemission spectroscopy [20]. In [8] we generalized the local constraint associated with (1) to $\chi_i^{00} + \chi_i^{\mu\mu} = N$, where N is an arbitrary integer, and considered the commutation properties of the χ^{ab} operators to be those of the generators of the $U(3)$ algebra. A generalized Holstein–Primakoff realization for the latter algebra reads

$$\begin{aligned} \chi_i^{00} &= N - \xi_i^{\mu*} \xi_i^\mu & \chi_i^{\mu\nu} &= \xi_i^{\mu*} \xi_i^\nu \\ \chi_i^{0\mu} &= (N - \xi_i^{\nu*} \xi_i^\nu)^{1/2} \xi_i^\mu & \chi_i^{\mu 0} &= \xi_i^{\mu*} (N - \xi_i^{\nu*} \xi_i^\nu)^{1/2} \end{aligned} \quad (3)$$

where the ξ_i^μ are Bose operators, $[\xi_i^\mu, \xi_j^{\nu*}] = \delta_{ij} \delta^{\mu\nu}$. Note that the local constraint, giving rise to the hard-core character of the bosons, has been explicitly resolved in (3). One can then develop a perturbation theory based on the $1/N$ expansion, restoring the relevant physical value $N = 1$ at the end of the calculation.

In the presence of an external magnetic flux Φ , threading the two-dimensional lattice in an Aharonov–Bohm torus geometry, the hopping matrix elements t_{ij} are modified by the well known Peierls phase factor and should be substituted in (1) according to

$$t_{ij} \rightsquigarrow t_{ij} e^{iA_{ij}} \quad \text{with } A_{ij} = \frac{2\pi\Phi}{\Lambda_x\Phi_0}(\mathbf{R}_i - \mathbf{R}_j) \cdot \mathbf{e}_x. \quad (4)$$

Here \mathbf{R}_i is the position vector for site i , \mathbf{e}_x is the unit vector along the x -axis encircling the flux lines and $\Phi_0 = 2\pi\hbar c/q$ is the so-called flux quantum. Conventionally, the charge q of the carriers entering Φ_0 is, of course, equal to the electronic charge e . However, the arguments of Thouless [7] quoted in the introduction imply that a vacancy actually ‘feels’ twice as much external flux. In the context of the present *effective* model this may be accounted for by an extra factor of two in the expression (4) for the A_{ij} , which can be readily absorbed in a redefinition of q as $q = 2e$. Evidently, this reasoning does not constitute a rigorous justification for the assignment $q = 2e$ in the flux quantum Φ_0 . The latter justification can be provided only by an *ab initio* derivation of an effective Hamiltonian for the hard-core boson vacancies, starting from a realistic electronic model for the cuprates. At present such a program is out of reach. Hence this work will be content with the study of the flux quantization properties of the effective model described by (1)–(4), given the flux quantum constant Φ_0 .

In the large- N limit ‘condensation’ occurs, i.e. the Bose operators ξ_i^μ , $\mu = 1, 2$, become classical commuting fields. For uniform density states these complex number amplitudes may then be parametrized as

$$\begin{aligned} \xi_i^1 &= \sqrt{Nn_e} \cos\left(\frac{\theta_i}{2}\right) e^{i\psi_i/2} e^{-i\phi_i/2} \\ \xi_i^2 &= \sqrt{Nn_e} \sin\left(\frac{\theta_i}{2}\right) e^{i\psi_i/2} e^{i\phi_i/2} \end{aligned} \quad (5)$$

where n_e is the average electronic density, the angles θ_i and ϕ_i determine the local spin direction, while the remaining parameter ψ_i determines the local phase of the condensate. As shown in [8], close to half-filling ($n_e \lesssim 1$) and for a sufficiently large t' , the ground state of (1) is described by a planar spin configuration ($\theta_i = \pi/2$) in which the local twist angles *and* phases are modulated according to

$$\phi_i = \mathbf{Q} \cdot \mathbf{R}_i \quad \psi_i = \mathbf{Q}' \cdot \mathbf{R}_i \quad (6)$$

where $\mathbf{Q} = (\pi, \pi)$ is the usual spin-modulating antiferromagnetic wavevector and $\mathbf{Q}' = (\pi, -\pi)$ is an unusual phase-modulating wavevector. We should note here that the excitation spectrum above this ground state is gapless [8], hence, as quoted in the introduction, the limiting value of the optical conductivity $\sigma(\omega \rightarrow 0)$ remains finite, at finite hole doping. However, as the half-filled-band limit is approached ($n_e \rightarrow 1$) the quantity $\sigma(\omega \rightarrow 0)/(1 - n_e)$ becomes increasingly depressed [9]. This trend is consistent with the ubiquitous ‘pseudogap’ behaviour observed in the optical and magnetic properties of underdoped cuprates [21] and provides further support to the relevance of the metallic phase-modulated antiferromagnetic (AF) ground state under consideration. The question that is now posed is how this ground state will respond to the presence of an external magnetic flux Φ .

3. Flux quantization and superfluid weight

Following an argument by Yang [22] we note that, in the presence of Φ , the reciprocal lattice is displaced from the origin by $2\pi\Phi/(\Lambda_x\Phi_0)$ along the x -axis. The quantization of

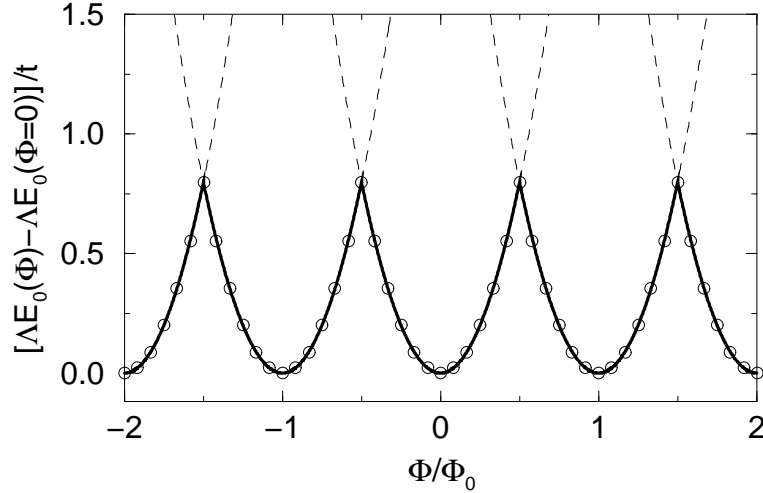


Figure 1. Ground-state energy versus external magnetic flux, for $\varepsilon = 0.45$, $t/J = 1.0$ and $1 - n_e = 0.10$. The zero-flux energy is subtracted to normalize the values. Solid line: the analytic result in the infinite lattice limit ($\Lambda \rightarrow \infty$), according to equations (8)–(9). Dashed lines: remnants of the crossing energy-level parabolas discussed in the text. Open circles: numerical minimization results for the ground-state energy on a finite lattice ($\Lambda = 20 \times 20$), as determined by equations (10) and (11). Evidently, the finite lattice numerical data (open circles) confirm the infinite lattice limit analytic result (solid line).

flux therefore depends on whether the ground-state energy of the system changes under this momentum boost. Given that the spin-exchange part of the Hamiltonian (1)–(4) does not couple directly to the magnetic flux it is plausible that, at least in the large- N limit, the condensate will respond in such a way as to leave its spin-modulating wavevector \mathbf{Q} intact and simply adjust its phase-modulating wavevector \mathbf{Q}' to a new value. In other words, we anticipate that, in this classical (large- N) limit, the rigidity of the ground state against the intrusion of the external magnetic flux comes solely from the phase fluctuations of the condensate. These heuristic arguments lead us to consider the *ansatz* (6) with the following modulating wavevectors

$$\mathbf{Q} = (\pi, \pi) \quad \mathbf{Q}' = (\pi, -\pi) - \left(\frac{4\pi m}{\Lambda_x}, 0 \right) \quad (7)$$

where m is an arbitrary integer. Inserting (7) into (5) and (6), the Hamiltonian (1)–(4) takes the form $H(\Phi) = N^2 \Lambda E_0(\Phi)$, where $E_0(\Phi)$ is the classical energy per lattice site for the value of physical interest $N = 1$. More explicitly, taking carefully the infinite lattice limit ($\Lambda \rightarrow \infty$) we have that

$$\Lambda E_0(\Phi) - \Lambda E_0(\Phi = 0) = 8t'\pi^2 n_e (1 - n_e) \left(\frac{\Phi}{\Phi_0} - m \right)^2. \quad (8)$$

Thus for each integer m we obtain an individual many-body energy level that depends quadratically on Φ . The ground-state energy is given by the lower envelope of these crossing energy-level parabolas and is characterized analytically by the condition

$$\left| \frac{\Phi}{\Phi_0} - m \right| \leq \frac{1}{2} \quad \text{with } m = 0, \pm 1, \pm 2, \dots \quad (9)$$

In figure 1 we depict by a solid line the ground-state energy calculated according to (8) and (9), for typical values of the parameters $\varepsilon = t'/t$, t/J and the hole concentration $(1 - n_e)$. We also depict by dashed lines the remnants of the individual crossing energy levels (8). Evidently, the ground-state energy (solid line) is an even periodic function of the external magnetic flux Φ , with a macroscopic energy barrier between different flux minima, in accordance with the Byers and Young [23] characterization of a superconductor. The period is equal to Φ_0 and therefore the assignment $q = 2e$, discussed earlier on, leads to agreement with the observed flux quantization in the high- T_c superconducting copper oxide layers [24]. In order to establish firmly the analytic result (8) and (9), and thus the heuristic arguments involved in (6) and (7), we have also minimized numerically the classical energy $\Lambda E_0(\Phi)$ obtained by inserting directly (5) into (1)–(4),

$$\Lambda E_0(\Phi) = \mathcal{E}_1 + \mathcal{E}_2 \quad (10)$$

where

$$\begin{aligned} \mathcal{E}_1 = & -n_e(1 - n_e) \sum_{i,j} t_{ij} \left[\cos \frac{\theta_i}{2} \cos \frac{\theta_j}{2} \cos \left(A_{ij} + \frac{\psi_i - \psi_j - \phi_i + \phi_j}{2} \right) \right. \\ & \left. + \sin \frac{\theta_i}{2} \sin \frac{\theta_j}{2} \cos \left(A_{ij} + \frac{\psi_i - \psi_j + \phi_i - \phi_j}{2} \right) \right] \\ \mathcal{E}_2 = & \frac{n_e^2}{4} J \sum_{(i,j)} [\cos \theta_i \cos \theta_j + \sin \theta_i \sin \theta_j \cos(\phi_i - \phi_j) - 1]. \end{aligned} \quad (11)$$

The minimization of (10) and (11) was carried out by a relaxation method. Excellent agreement with the analytic result (8) and (9) was obtained even for lattices with $\Lambda = 20 \times 20$, and for all choices of the parameters ε , t/J and n_e , within the range of stability of the phase-modulated AF ground state. A specific example of this agreement is evidenced in figure 1, where the open circles correspond to the numerical minimization data.

Let us now turn our attention to the superfluid weight (or helicity modulus) D_s given by the curvature of the infinite lattice limit of the ground-state energy $\Lambda E(\Phi)$ at $\Phi = 0$ [22, 23, 25],

$$D_s = \Lambda \left(\frac{\Phi_0}{2\pi} \right)^2 \left[\frac{\partial^2 E(\Phi)}{\partial \Phi^2} \right]_{\Phi=0}. \quad (12)$$

D_s determines the ratio of the density of the superfluid charge carriers to their mass, and is related to the directly measurable in-plane London penetration depth λ_L by $D_s = c^2/(4\pi e^2 \lambda_L^2)$. Quite generally, $E(\Phi)$ has a $1/N$ expansion of the form $E(\Phi) = N^2 E_0(\Phi) + N E_1(\Phi) + \dots$ which leads via (12) to a corresponding expansion for the superfluid weight $D_s = N^2 D_s^{(0)} + N D_s^{(1)} + \dots$. Hence by exploiting the large- N limit result (8) and (9) we obtain immediately the expression for the leading term $D_s^{(0)}$,

$$D_s^{(0)} = 4t'n_e(1 - n_e). \quad (13)$$

Our earlier arguments show that $D_s^{(0)}$ is a measure of the stiffness of the classical phase fluctuations of the condensate. Furthermore, (13) implies $D_s^{(0)} = D_0$, where D_0 is the leading term in the $1/N$ expansion of the Drude weight $D = N^2 D_0 + N D_1 + \dots$, studied in [10] using the Kubo formalism for the current-current correlations. We have also verified, by a straightforward but lengthy calculation of $E_1(\Phi)$ and the use of (12), that $D_s^{(1)} = D_1$. Due to the analytic structure of the $1/N$ expansion, these results signify the term-by-term validity of the identity $D_s = D$. Strictly speaking, of course, we have checked explicitly that $D_s = D$ only up to and including terms $D_s^{(1)} = D_1$, i.e. only up to and including leading quantum-fluctuation effects [26]. This, however, is sufficient for most practical purposes

and permits us to exploit our calculations of the Drude weight, in the present study of the superfluid weight. For instance, the weight $D_s = D$, including leading quantum-fluctuation effects, is found [10] to increase linearly with small hole concentration ($1 - n_e$) away from the half-filled-band limit ($n_e = 1$). This trend, present already in (13), is a fundamental characteristic of doped antiferromagnets. At higher doping values $D_s = D$ eventually saturates and then starts to decrease. Note that the vanishing overlap between the opposite sublattice spin states, along with the absence of quantum fluctuations in the large- N limit, leaves the direct hopping t' between same sublattice sites as the only relevant process of charge transport in this classical approximation. This argument makes plausible the independence of $D_s^{(0)}$ from t and J seen in (13). However, the leading quantum-fluctuation correction $D_s^{(1)} = D_1$ involves already a non-trivial dependence on the latter couplings.

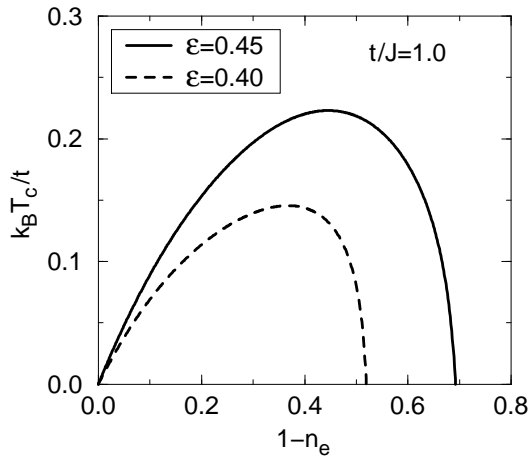


Figure 2. Superconducting transition temperature versus hole concentration, for $t/J = 1.0$ and $\varepsilon = 0.45$ (solid line) or $\varepsilon = 0.40$ (dashed line), according to equation (14) with the inclusion of leading quantum-fluctuation effects.

It should be noted that when $t' = 0$, the present model reduces to the simple t - J model where in the physically relevant regime, i.e. close to half-filling, the uniform density state under study becomes unstable against phase separation into an insulating (hole-poor) antiferromagnetic region and a conventional metallic (hole-rich) ferromagnetic region [27]. In the latter phase-separated state no flux quantization and finite superfluid weight occurs. A vanishing superfluid weight has been suggested also by the quantum Monte Carlo studies of the simple Hubbard model [25], although the corresponding exact-diagonalization studies of the fermionic t - J model [15] are not conclusive close to half-filling, due to the very small lattice sizes (e.g., 4×4) used. Indeed, the finite-size effects in the numerical studies of the latter system are particularly large because of the presence of phase separation in the ground state [28]. Our observations here underline the importance of the next-nearest-neighbour hopping t' to the ability of the mobile holes in sustaining a uniform density state that displays flux quantization and a finite superfluid weight. In this respect it is useful to recall that the effective hopping parameter t' accounts for the large oxygen-oxygen overlap integrals present in the original CuO_2 planes [18–20].

We will complete our report with a discussion of the expected transition temperature to the charged superfluid, i.e. superconducting, state under study. At a finite temperature T , the ratio of the thermal de Broglie wavelength of the charge carriers to their average distance is proportional to $\sqrt{D_s/(k_B T)}$, where D_s is the zero-temperature value determined by (12). Hence a naive application of the criterion for the occurrence of Bose-Einstein

condensation in an ideal boson gas, whereby the latter ratio should become of order unity, suggests a transition temperature T_c of the form

$$k_B T_c = A D_s \quad (14)$$

where A is a dimensionless constant of order unity. Of course, in the strictly two-dimensional model of continuous symmetry under study, a *bona fide* finite temperature phase transition can only be of the Kosterlitz–Thouless type which, nevertheless, leads again to an expression of the form (14). Indeed, the ψ_i -structure of the classical Hamiltonian (10) and (11) is a generalization of the two-dimensional XY model where the latter transition is well studied. In this context, it is important to note that a ‘universal’ linear relation of the form (14) has been established experimentally in the cuprates by Uemura *et al* [16] in their remarkable study of T_c as a function of the zero-temperature value of $\lambda_L^{-2} \propto D_s$. In the large- N limit, the D_s appearing in (14) is just equal to $D_s^{(0)}$ and the corresponding critical temperature $T_c^{(0)}$ should be interpreted as the ordering temperature for the classical phase fluctuations of the condensate, in analogy with the analysis of Emery and Kivelson [29] of the classical phase fluctuations of the conventional BCS order parameter. The higher order terms in the $1/N$ expansion of $D_s = D$ capture the effects of the quantum fluctuations and renormalize downwards these weights [10], thereby reducing the corresponding value of T_c .

Following the prescription of Emery and Kivelson [29], we have applied (14) with $A = 0.9$, a numerical value extracted from the two-dimensional XY model [30]. Using the calculated $D_s = D$ of [10], with the inclusion of the leading quantum-fluctuation correction $D_s^{(1)} = D_1$, we depict in figure 2 the superconducting transition temperature T_c as a function of the hole concentration $(1 - n_e)$. Evidently, the dependence of T_c on $(1 - n_e)$ reflects that of D_s and reproduces qualitatively the observed trends in the cuprates [16, 17]. With an estimated $J/k_B \approx 1500$ K in the latter materials [31], the value of T_c at optimum doping $(1 - n_e) = 0.44$ (0.36), seen in the solid (dashed) line of figure 2, is $T_c \approx 335$ K (218 K). This predicted value of T_c , signalling the coherence of the phase fluctuations of the condensate, should be regarded as an upper bound to an actual transition temperature because of the neglect of impurity disorder, higher-order quantum fluctuations etc. From figure 2 we also note that with further hole doping T_c starts to decrease while beyond a critical doping value it vanishes, as the phase-modulated AF configuration, around which the present $1/N$ expansion is carried out, becomes unstable.

4. Conclusions

In this paper, we have demonstrated that flux quantization and a concomitant finite value of superfluid weight D_s occur in the metallic phase-modulated AF ground state of the t - t' - J model (1). The classical phase fluctuations of the condensate are shown to control the leading term in the $1/N$ expansion of D_s . By appealing to the universality class of the two-dimensional XY model, the corresponding superconducting transition temperature T_c is related to D_s linearly, via (14). The inclusion of leading quantum-fluctuation effects in D_s provides then a reasonable estimate for the order of magnitude and the doping dependence of T_c in the cuprates. The latter dependence is of particular importance as it emerges from a consistent many-body $1/N$ expansion that preserves, at each order of perturbation theory, the local constraint, implied by the strong-correlation effects. These results support our effective description of the charge carriers in terms of hard-core bosons.

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