Properties of conduction-band dilute-magnetic-semiconductor quantum wells in an in-plane magnetic field: A density of states profile that is not steplike

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We examine how an in-plane magnetic field B modifies the density of states (DOS) in narrow-to-wide, conduction-band dilute-magnetic semiconductor quantum wells. We demonstrate that the DOS diverges significantly from the *ideal* steplike two-dimensional electron gas form and this causes severe changes to the physical properties, e.g., to the spin-subband populations, the internal and free energy, the Shannon entropy, and the in-plane magnetization M. We predict a considerable fluctuation of M in cases of vigorous competition between spatial and magnetic confinement.

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When a magnetic field B is applied parallel to a quasi-two-dimensional electron gas (2DEG) layer, an interplay between spatial and magnetic localization is established. In the general case, it is necessary to compute self-consistently the energy dispersion.[1,2] In a dilute magnetic semiconductor (DMS) structure, due to the enhanced energy splitting between spin-up and spin-down states, all possible degrees of freedom become evident, and the density of states (DOS) acquires the form

$$n(\mathcal{E})=\frac{A\sqrt{2m^*}}{4\pi^2\hbar}\sum_{i,\sigma}\int_{-\infty}^{+\infty}dk_x\frac{\Theta(\mathcal{E}-E_{i,\sigma}(k_x))}{\sqrt{\mathcal{E}-E_{i,\sigma}(k_x)}}. \qquad (1)$$

The quasi-2DEG layer is parallel to the xy plane and B is applied along the y axis. Θ is the step function, A is the xy area of the structure, m^* is the effective mass, and $E_{i,\sigma}(k_x)$ are the spin-dependent xz plane eigenenergies which must be self-consistently calculated. Equation (1) is valid for any type of interplay between spatial and magnetic localization, i.e., for *narrow* as well as for *wide* quantum wells (QW's). In the limit $B\to 0$, the DOS retains the *famous* (and occasionally stereotypic) steplike 2DEG form. Another asymptotic limit of Eq. (1) is that of a simple saddle point, where the DOS diverges logarithmically.

Considerable advance has been achieved for III-V-based magnetic semiconductors which utilize the valence band[3] e.g., (In,Mn)As and (Ga,Mn)As. In view of that, we examine a system where conduction-band spintronics can be achieved; specifically we analyze n-doped *narrow*-to-*wide* DMS ZnSe/$Zn_{1-x-y}Cd_xMn_ySe$/ZnSe QW's. A principal reason which increases the influence of B and drives this system away from the parabolic dispersion is the relatively low conduction-band offset ΔE_c. We use $\Delta E_c = 1$ Hartree*.[4] In the present system the *enhanced* electron spin-splitting $U_{o\sigma}$ is not proportional to the cyclotron gap, $\hbar\omega_c$, i.e., $U_{o\sigma} = (g^*m^*/2m_e)\hbar\omega_c + N_0\eta y(5/2)B_{5/2}(\xi) = \alpha+\beta$.[4] g^* is the effective Landè factor and m_e is the electron mass. The term β arises from the exchange interaction between the conduction electron and the Mn^{+2} cations. N_0 is the concentration of cations and η is the expectation value of the exchange coupling integral over a unit cell. $N_0\eta y$ ($y=0.035$) is taken 0.13 Hartree*.[4] $B_{5/2}(\xi)$ is the standard Brillouin function. ξ is a quantity with denominator k_BT and numerator containing two terms: the first one includes B, and the second one includes the difference between spin-up and spin-down populations.[5,6] T is the temperature and k_B is the Boltzmann constant. In the present paper $T=4.2$ K, thus $B_{5/2}(\xi)\simeq 1$. Hence, $\beta=0.325$ Hartree*. For ZnSe, $\alpha\approx\tau 10^{-3}$ Hartree*, where τ is the arithmetic value of B in Tesla. The term α is one or two orders of magnitude smaller than the term β. Therefore, it is convenient in the *first approximation* to ignore α. For ZnSe, 1 Hartree*$\approx$70.5 meV, thus $\beta\approx 23$ meV. The electronic states' calculation and the material parameters can be found elsewhere.[7,8] Due to the numerical cost, the k_x dependence is often ignored.[4,6] However, this is adequate only if the spatial localization dominates.

The DOS is the *core* of the system and its changes affect all physical properties. If $f_0(\mathcal{E})$ is the Fermi-Dirac distribution, the total electron population, $N=\int_{-\infty}^{+\infty}d\mathcal{E}n(\mathcal{E})f_0(\mathcal{E})$, the internal energy, $U=\int_{-\infty}^{+\infty}d\mathcal{E}n(\mathcal{E})f_0(\mathcal{E})\mathcal{E}$, and the Shannon entropy,[9] $S=-k_B\int_{-\infty}^{+\infty}d\mathcal{E}n(\mathcal{E})f_0(\mathcal{E})\ln[f_0(\mathcal{E})]$. Hence, N, U, and S, can be calculated.[10] Qualitatively, if N is kept constant, we expect that $|U|$ will decrease whenever B induces flattening of the occupied spin-subbands, since this leads to occupied energies with smaller $|\mathcal{E}|$. On the other hand, S is sensitive to the changes of $\ln[f_0(\mathcal{E})]$. At $T=4.2$ K, these changes only occur in a short region around the chemical potential $\mu\equiv 0$. In other words, S *reads* the modification of the dispersion around $\mu\equiv 0$. The free energy $F=U-TS$. The main contribution to F—at this low T—comes from U. The in-plane magnetization, $M=-(1/V)(\partial F/\partial B)_{N,T}$, where V is the structure's volume. In the following, we deliberately keep T and N constant (we assume that all donors—e.g., Cl—are ionized). $N/A = 1.566\times 10^{11}$ cm^{-2}. We symbolize 00 the ground-state spin-down-subband, 10 the first excited spin-down subband, 01 the ground-state spin-up subband, and finally 11 the first excited spin-up subband. To illustrate the antagonism between the spatial and the magnetic confinement we present results corresponding to different well widths L, i.e., 10 nm, 30 nm, and 60 nm. As a *unit* of DOS we use the ideal 2DEG step, $(m^*A)/(\pi\hbar^2)$.

For $L=10$ nm, the spatial confinement dominates. Even for $B=20$ T, the $E_{i,\sigma}(k_x)$ retain a "parabolic shape" and the

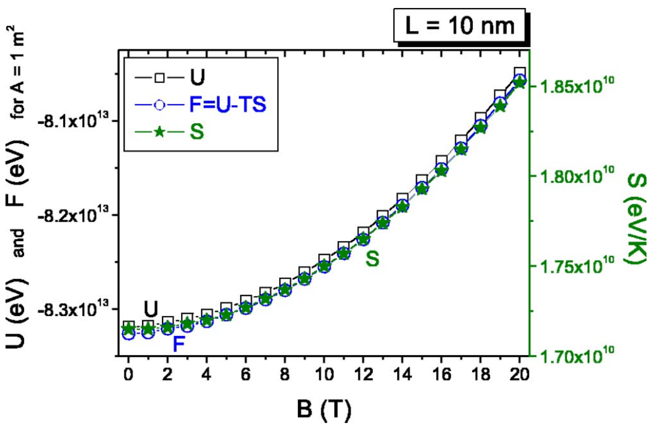

FIG. 1. (Color online) $L=10$ nm. Internal energy U, free energy F, and entropy S, as a function of B. The dispersion is *almost parabolic* and increase of B induces a slight flattening of the spin subbands.

DOS is an almost "perfect staircase" with steps increasing $\sim 7.5\%$ for the 00 spin subband and $\sim 10\%$ for the 01 spin subband, relatively to the ideal 2DEG step. This increase is due to the B-induced slight flattening of the $E_{i,\sigma}(k_x)$. Only 00 is occupied. Figure 1 depicts U, F, and S as a function of B in the range 0–20 T. All these physical properties exhibit "a single behavior" because the system has "almost parabolic" spin subbands.

Figures 2 and 3 demonstrate how the ideal picture is modified for $L=30$ nm. Figure 2 presents the $E_{i,\sigma}(k_x)$ and the DOS for characteristic values of B. Even for $B=4$ T, since the $E_{i,\sigma}(k_x)$ are no longer "perfect parabolas," there is a quantitative modification of the DOS. For $B=6$ T there are two impressive singularities and the DOS is quantitatively different from the ideal 2DEG staircase. Figure 3 depicts the spin-subband sheet electron populations, N_{ij}, as well as U, F, and S as a function of B in the range 0–20 T. For $B=0$ there are two populated spin subbands i.e., $N_{00}=1.397\times 10^{11}$ cm^{-2} and $N_{10}=0.169\times 10^{11}$ cm^{-2}. In the region 0–6 T, we observe the gradual *depopulation* of the 10 spin subband. During this process, the perfect parabola is slightly distorted and the 10 partial DOS for $B=6$ T looks like an "old abraded step." In the region 4–12 T the 00 and 01 spin subbands change drastically, i.e., from almost parabolic with a single minimum gradually develop a two-minima shape. This is characteristically mirrored in the submersion of U and F. For $B\geqslant 12$ T the dispersion retains the two-minima shape, while the basic effect of increasing B is the decrease of the electron concentration in the center of the well. As discussed above, S is very sensitive to these dispersion modifications. S clearly exhibits [Fig. 3(b)] "three distinct behaviors" approximately in the zones 0–4 T (concave down), 4–12 T (concave up), and 13–20 T (concave down). For the whole range 0–20 T, N is made up only from spin-down carriers. Even if some spin-up electrons survived, we could in principle utilize the effect of *depopulation* of the higher spin subbands to eliminate spin-up electrons.

Let us now consider a wider QW with $L=60$ nm. For $B=0$, the partial DOS of all spin subbands is exactly 0.5 ideal 2DEG step. The 00—10 parabolas as well as the 01—11 parabolas are energetically very close. The resulting populations are $N_{00}=7.934\times 10^{10}$ cm^{-2}, $N_{10}=7.726\times 10^{10}$ cm^{-2}, $N_{01}=5.009\times 10^{-15}$ cm^{-2}, and $N_{11}=4.316\times 10^{-15}$ cm^{-2}, i.e., only spin-down electrons survive. Only 10 has some population in the center of the well but the system is basically already a bilayer one. Figure 4 presents the $E_{i,\sigma}(k_x)$ and the DOS for $L=60$ nm and characteristic values of B. The ideal steplike DOS cannot describe the system even for relatively small B. For $B=2$ T the two pairs of dispersion

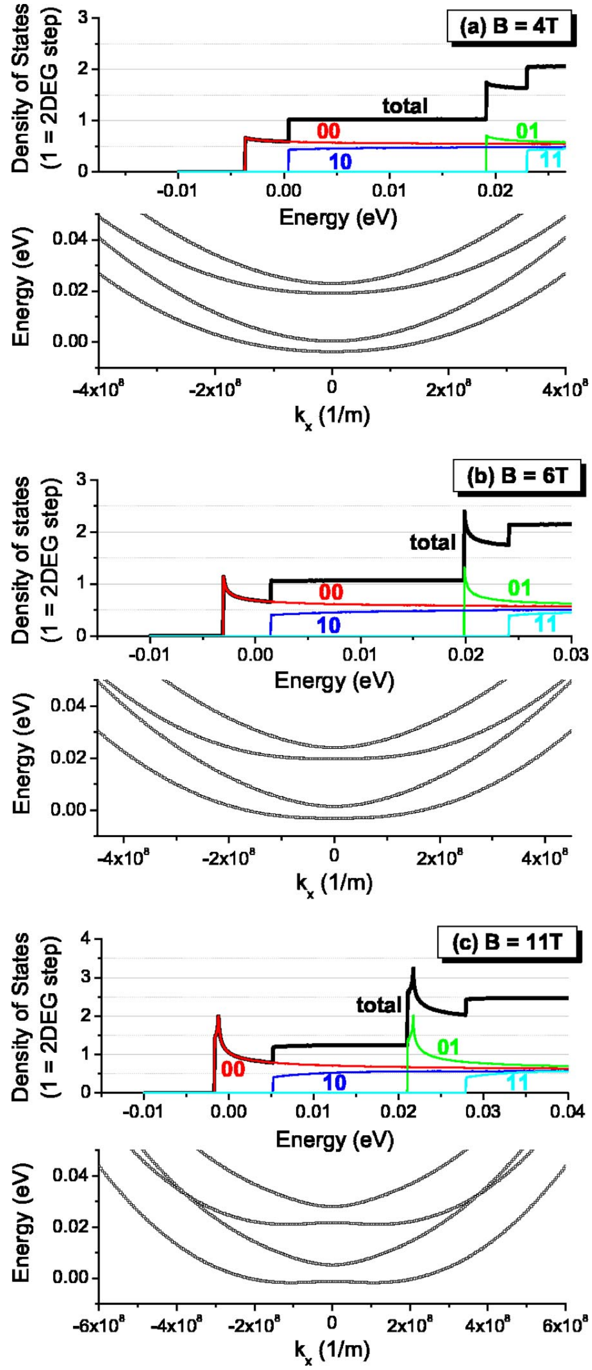

FIG. 2. (Color online) $E_{i,\sigma}(k_x)$ and DOS for $L=30$ nm. (a) $B=4$ T, (b) $B=6$ T, and (c) $B=11$ T. In the region 4–12 T the 00 and 01 spin subbands change drastically, gradually developing a two-minima shape.

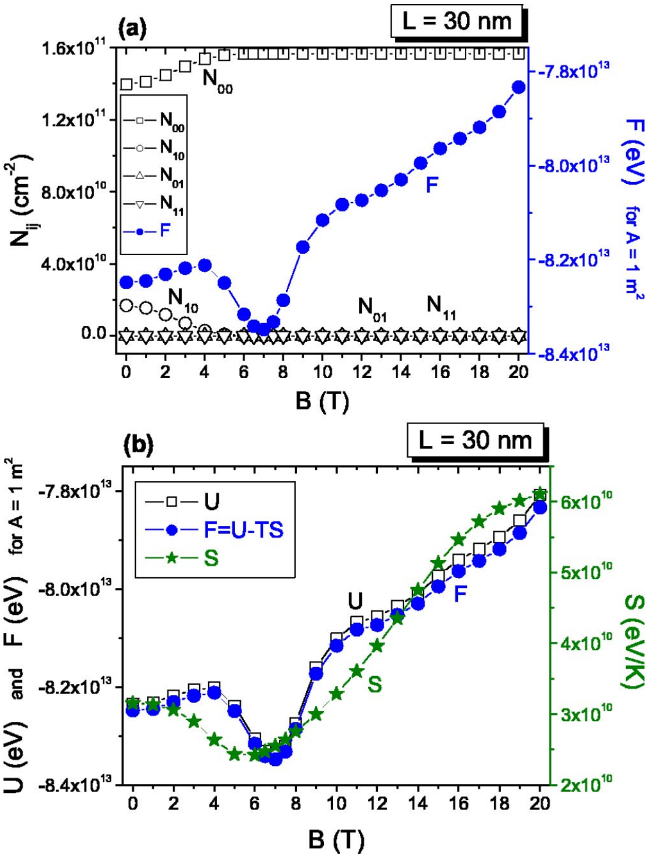

FIG. 3. (Color online) $L=30$ nm. (a) Spin-subband sheet electron populations N_{ij}, and free energy F; (b) internal energy U, free energy F, and entropy S, as a function of B. The drastic dispersion modification is mirrored in the behavior of U, F, and S.

curves corresponding to spin-down and spin-up electrons anticross at $k_x=0$ and the total DOS has been already slightly modified. For $B=7$ T some nice singularities are present while the shape and magnitude of the DOS is far away from the famous 2DEG staircase. For $B=20$ T the $k_x=0$ energy separation of the members of the spin-up and spin-down pairs is 14.11 meV $\simeq\hbar\omega_c=14.47$ meV. Hence, in the center of the well the magnetic confinement has overcome the spatial confinement. In this region, the DOS is that of a free particle along the y axis plus a harmonic oscillator in the xz plane. Figure 5 presents N_{ij}, as well as U, F, and S, as a function of B in the range 0–20 T. Initially, in the zone 0–4 T, the magnetic field depopulates the 10 spin subband. During this process the 10 dispersion retains a ''one minimum'' form. In the 0–4 T range, the dispersion loses gradually the two-parabolas' type, developing via anticrossing the two-minima shape in the 00 spin subband. In the 4–20 T range, only the 00 spin subband remains populated retaining the two-minima shape. These two types of behavior can be seen in the modification of U and F. Again, more sensitive to these dispersion modifications is S, which is concave up in the 0–4 T range but an absolutely straight line in the range 4–20 T!

Using a derivative algorithm we obtain the in-plane magnetization (Fig. 6). Since L is different in these three cases, we present the product magnetization times volume MV, in

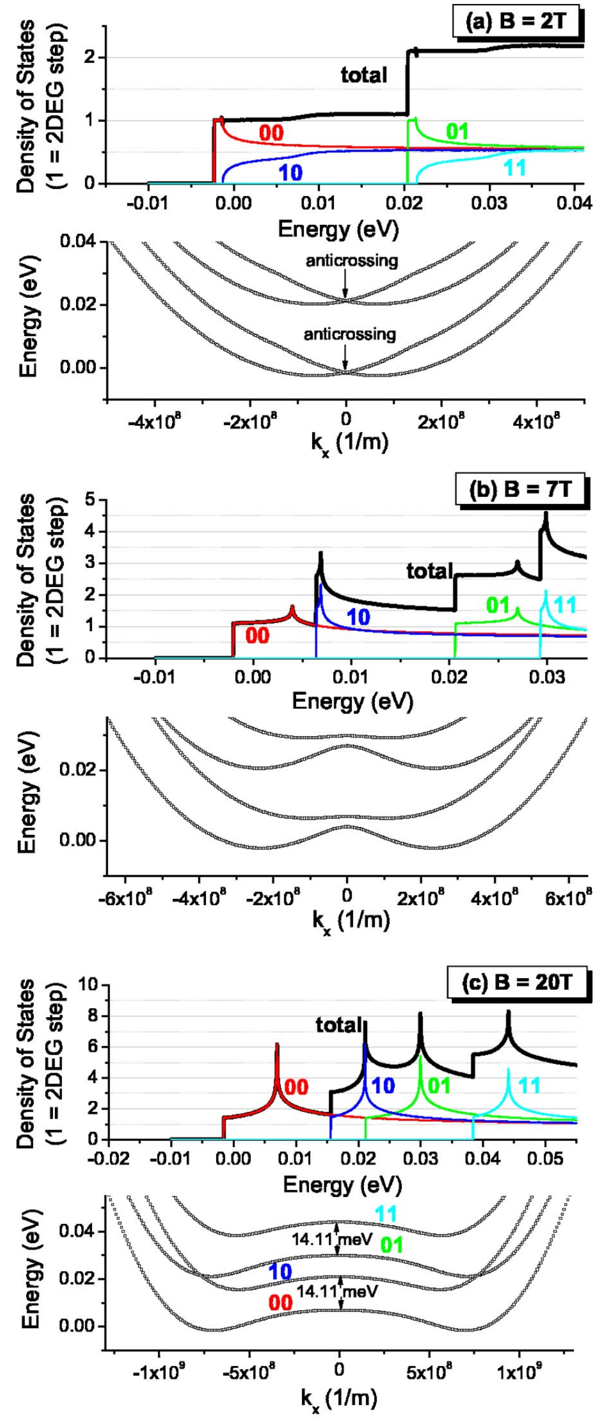

FIG. 4. (Color online) $E_{i,\sigma}(k_x)$ and DOS for $L=60$ nm. (a) $B=2$ T, (b) $B=7$ T, and (c) $B=20$ T. This is basically a spin-down bilayer system.

units of eV/T instead of M alone. For $L=10$ nm there is a simple almost straight line because the dispersion remains ''basically parabolic.'' For $L=60$ nm, since the structure ''is basically a bilayer system'' no big surprises are present. The situation is different for $L=30$ nm. Here, in the region where the dispersion changes drastically, we observe a severe fluctuation of M, which is so big that the lines for $L=10$ nm and $L=60$ nm seem almost constant. The magnitude of the magnetization fluctuation—for this 30 nm

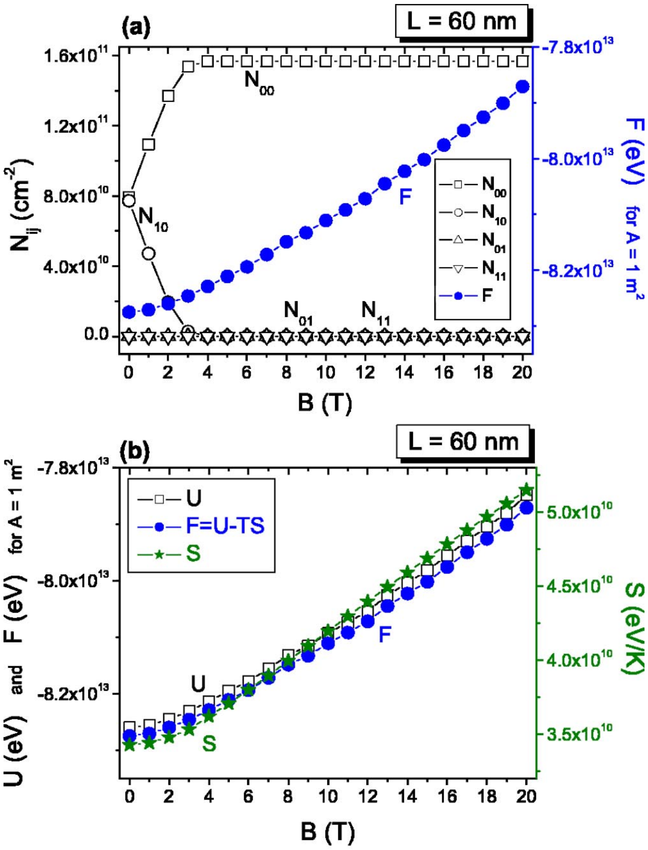

FIG. 5. (Color online) $L=60$ nm. (a) Spin-subband sheet electron populations N_{ij} and free energy F; (b) internal energy U, free energy F, and entropy S, as a function of B. The two "dispersion zones," 0–4 T and 4–20 T, are mirrored in the behavior of U, F, and S.

well—is $\approx 5\ \mathrm{Am}^{-1}$. This corresponds $\sim$ to a Mn concentration of $10^{17}\ \mathrm{cm}^{-3}$. Conclusively, the DOS modification has caused an impressive effect on the system's in-plane magnetization.

To our knowledge, there has been no experimental study of the present system under in-plane magnetic field. We note two photoluminescence studies performed in the Faraday geometry, with the magnetic field applied perpendicular to the layers: one of the narrow QW at 4.2 K (Ref. 11) and one of the asymmetric double QW at 1.8 K.[12] Interesting magnetic/nonmagnetic structures with different layers of ZnCdSe, ZnSe, and ZnCdMnSe have been magneto-optically investigated more recently,[13,14] without taking advantage of a parallel magnetic field. Hence, in order to exploit the potentialities of the present system we would like to encourage experiments with in-plane magnetic field and wider quantum wells.

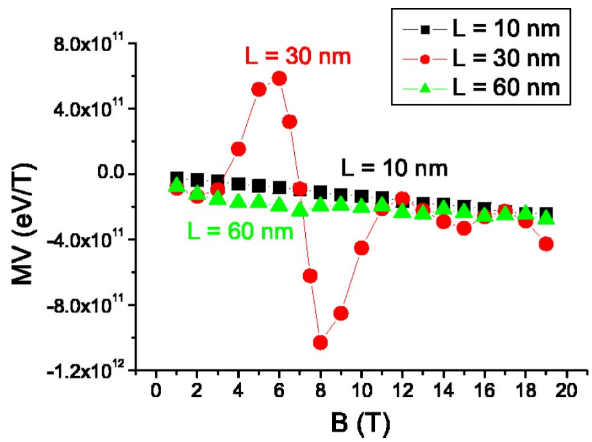

FIG. 6. (Color online) In-plane magnetization times volume MV, as a function of B. Note the fluctuation for $L=30$ nm due to the severe DOS modification.

We have illustrated—by providing results for different degrees of magnetic and spatial confinement—how much the *classical* staircase 2DEG density of states must be modified, for n-doped $ZnSe/Zn_{1-x-y}Cd_xMn_ySe/ZnSe$ QW's, under in-plane magnetic field. This is a valuable system for conduction-band spintronics. The DOS modification causes considerable effects on the system's physical properties. We have described the changes induced to the spin-subband populations, the internal and free energy, the entropy, and the in-plane magnetization. We predict a significant fluctuation of the in-plane magnetization when the dispersion is severely modified by the parallel magnetic field.

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