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## Oscillatory effects and the magnetic susceptibility of carriers in inversion layers

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**Abstract.** Oscillatory effects in a strong magnetic field  $B$  and magnetic susceptibility are investigated, as applied to 2D systems, in which the twofold spin degeneracy is lifted by the spin-orbit-interaction Hamiltonian  $H_{SO} = \alpha(\boldsymbol{\sigma} \times \mathbf{k}) \cdot \boldsymbol{\nu}$ . The term  $H_{SO}$  is shown to change greatly the usual patterns of  $B^{-1}$ -periodic oscillations; some oscillations are strongly suppressed due to the diminishing of the gaps between adjacent levels, and new oscillations appear due to intersections of levels.

### 1. Introduction

Experimental data on the combined resonance (i.e., electric dipole spin resonance) and the cyclotron resonance of 2D electron gas (EG) at the interfaces of GaAs–Al<sub>x</sub>Ga<sub>1-x</sub>As heterojunctions, reported recently by Stein *et al* (1983) and by Stormer *et al* (1983) has unambiguously made manifest that the spin degeneracy is lifted in inversion layers. The dispersion law for carriers in such layers is unusual because of the existence of a ring of extrema (Rashba and Sheka 1959, Rashba 1961, Casella 1960) where the energy reaches minimum. The theory of electron resonances in 3D semiconductors with such spectra, developed earlier (Rashba 1960), enabled us (Bychkov and Rashba 1984) to describe from the same point of view the experimental data from the papers of Stein *et al* (1983) and Stormer *et al* (1983), and to determine the spin-orbit- (so-) coupling constant  $\alpha$ . The theory proposed is based on the following expression for a so Hamiltonian:

$$H_{SO} = \alpha[\boldsymbol{\sigma} \times \mathbf{k}] \cdot \boldsymbol{\nu}. \quad (1)$$

Here, the  $\boldsymbol{\sigma}$  are Pauli matrices and  $\boldsymbol{\nu}$  is a unit vector perpendicular to the surface. The operator  $H_{SO}$  lifts the twofold spin degeneracy at  $\mathbf{k} \neq 0$  and determines the so band splitting near  $\mathbf{k} = 0$ .

The possibilities for experimental studies of de Haas–van Alphen (dHvA) oscillations in 2D EG were demonstrated recently by Haavasaaja *et al* (1984) and by Fang and Stiles (1983). In this paper we investigate the general patterns of the oscillatory phenomena (dHvA and Shubnikov–de Haas (SdH) oscillations) in 2D systems with the so Hamiltonian (1). The magnetic susceptibility (MS) is investigated in more detail. These phenomena provide new possibilities for the independent determination of  $\alpha$ .

## 2. Energy spectrum and oscillatory phenomena

The effective-mass Hamiltonian with the spin-orbit term (1) has the form

$$H = \hbar^2 k^2 / 2m + \alpha [\boldsymbol{\sigma} \times \mathbf{k}] \cdot \boldsymbol{\nu}. \quad (2)$$

Here  $\mathbf{k}$  is the two-dimensional quasimomentum,  $k = |\mathbf{k}|$ . The energy spectrum consists of two branches:

$$E^{(\pm)}(k) = \hbar^2 k^2 / 2m \pm \alpha k. \quad (3)$$

The lower branch,  $E^-(k)$ , reaches a minimum on the ring (or the circle) of extrema, the radius of which is  $k_0 = \alpha m / \hbar^2$ .  $E^-(k_0) = -\alpha^2 m / 2\hbar^2 \equiv -\Delta$ .

The energy spectrum for a magnetic field  $B$  is determined by the formulae (Rashba 1960)

$$E_s^\pm = \hbar \omega \epsilon_s^\pm \quad \epsilon_0 = \delta \quad \epsilon_s^\pm = s \pm (\delta^2 + \gamma^2 s)^{1/2} \quad s \geq 1 \quad (4)$$

where the  $s$  are integers and

$$\omega = eB/mc \quad \gamma = 2(\Delta/\hbar\omega)^{1/2} \quad \delta = \frac{1}{2}(1 - mg/2m_0). \quad (5)$$

Here  $m_0$  is the mass of the free electron and  $g$  is the  $g$ -factor. Figure 1 shows the dispersion  $E^\pm(k)$  and figure 2 shows the function  $E_x^\pm$ , which can be obtained from  $E_s^\pm$  by substituting for the integer  $s$  with the arbitrary number  $x$ .

It is seen from figure 1 that there is a 'pocket' on the curve for  $E^-(k)$ —the region where  $E^-(k) < 0$ . Its radius is equal to  $2k_0$ , and it is completely occupied by EG at the concentration

$$n_{\text{cr}} = \alpha^2 m^2 / \pi \hbar^4 = \gamma^2 n_L \quad n_L = eB/hc \quad (6)$$

where  $n_L$  is the multiplicity of Landau levels (per unit area).

It follows from (4) that the energy levels of a 2D system in a magnetic field show some peculiarities. When the field is weak, i.e. when  $\gamma^2 \gg 1$  (or  $\hbar\omega \ll \Delta$ ), the quasiclassical description holds and the number of levels in the energy region where  $E_s^\pm \leq E$  is proportional to the corresponding area in the  $k_x k_y$ -plane. For example, the number of levels in the pocket outside the ring of extrema is three times as large as that inside the ring. When  $B$  increases, the levels move to the right along the curves  $E_s^\pm$  (figure 2). This

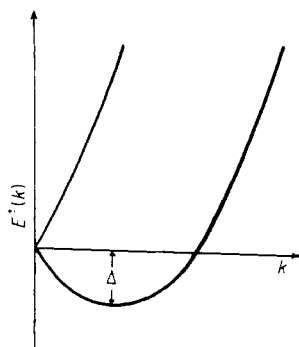


Figure 1. The dispersion law  $E^\pm(k)$ .

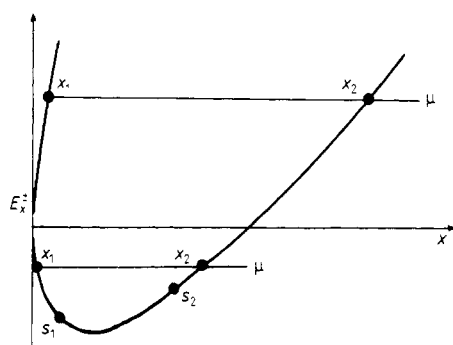


Figure 2. The function  $E_x^\pm$ .

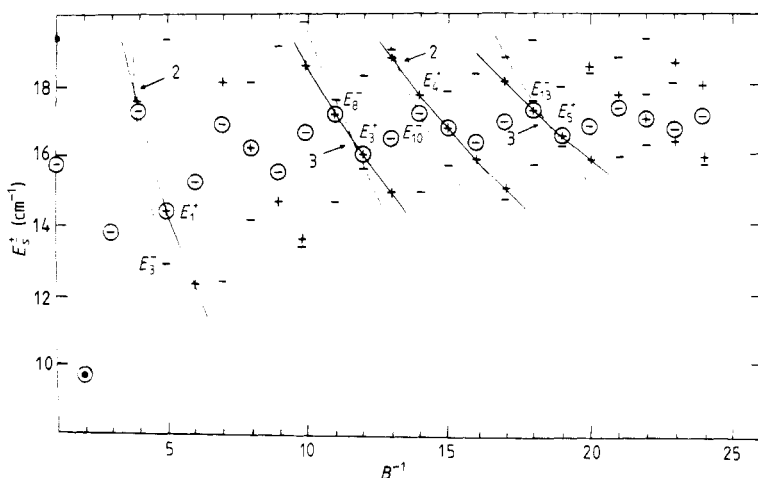
means that on the branch  $E^-$  the levels that are on the left (right) of point  $-\Delta$  move downwards (upwards); see, e.g., levels  $s_1$  and  $s_2$  in figure 2. As a result, the intersection of levels occurs at definite values of  $B$ . The same happens for  $E > 0$ . Despite the fact that with increasing  $B$  the levels move in the same direction, namely upwards, on both branches, the motion of levels proceeds faster along branch  $E^-$  than along  $E^+$ . Therefore the levels belonging to different branches also intersect.

It follows from (4) that if

$$s_0 - \delta^2/s_0 < \gamma^2 < s_0 + 1 - \delta^2/(s_0 + 1) \quad (7)$$

then for arbitrary  $B$  there are  $s_0$  negative eigenvalues on the branch  $E^-$ . Since usually  $\delta^2 \ll 1$ , it follows from (6) and (7) that the number of levels in the pocket is  $\approx \gamma^2 = n_{\text{cr}}/n_L$ . The last negative  $E^-$ -level leaves the pocket at  $\gamma_{\text{cr}}^2 = 1 - \delta^2 \sim 1$ .

Oscillatory effects (both dHvA and SdH oscillations) are determined by the dependence of energy levels on  $B$  and by the redistribution of carriers between various levels. When the term  $H_{\text{SO}}$  is absent, the period of oscillations is well known to be  $e/chn = B_0^{-1}$  in the  $B^{-1}$ -scale. However, the intersection of levels belonging to different branches mentioned above has to introduce new features into the oscillation patterns. To obtain a realistic picture of the energy spectrum and the occupancy of different levels, we have computed with the aid of (4) the position of the levels for the parameter values of the device used by Stormer *et al* (1983) in their investigation of SdH oscillations. These are  $m \approx 0.5 m_0$ ,  $n \approx 5 \times 10^{11} \text{ cm}^{-2}$ . From the cyclotron resonance data we have found  $\alpha = 0.6 \times 10^{-9} \text{ eV cm}$  and  $\Delta \approx 10^{-4} \text{ eV}$  (Bychkov and Rashba 1984). Hence,  $n = 10 n_{\text{cr}}$ . The value of  $\delta$  remains unknown, and we put  $\delta = 0.5$ ; this affects only the position of a few first levels. The position of levels in the vicinity of Fermi energy is shown in figure 3. In figure 3 and below in this section, the magnetic field  $B$  is measured in units of  $B_0 = 206 \text{ kG}$ ;  $B_0$  corresponds to the complete occupation of the first Landau level. Therefore, when  $B^{-1}$  is an integer, the  $B^{-1}$  lowest Landau levels are occupied and the other levels are empty (temperature  $T = 0$ ). The last occupied level is encircled in figure 3 for all integer values of  $B^{-1}$ . With increasing  $B^{-1}$  the occupation of the next level begins.



**Figure 3.** The positions of Landau levels near the Fermi energy versus the non-dimensional inverse magnetic field. +: the branch  $E^+$ ; -: the branch  $E^-$ ; ●: the level  $E_0$ . Full and broken curves connect + and - points, respectively.

When  $B^{-1}$  rises, three types of redistribution of carriers between Landau levels are possible, as is seen in figure 3.

*Case 1.* Each time that  $B^{-1}$  only slightly exceeds an integer, the level following the encircled one starts being filled. These two levels may belong to the same branch or to different branches. So, when  $5 < B^{-1} < 6$  the level  $E_4^-$  (following  $E_1^+$ ), when  $6 < B^{-1} < 7$  the level  $E_5^-$  (following  $E_4^-$ ) and when  $7 < B^{-1} < 8$  the level  $E_2^+$  (following  $E_5^-$ ) are being filled.

*Case 2.* A partly filled level intersects an empty level, belonging to the other branch. Two such intersections, at  $3 < B^{-1} < 4$  and  $13 < B^{-1} < 14$  are seen in figure 3. They are indicated by arrows marked with the number 2.

*Case 3.* A partly filled level intersects a totally occupied level, belonging to another branch. Two such intersections, at  $11 < B^{-1} < 12$  and  $18 < B^{-1} < 19$ , are seen in figure 3. They are indicated by arrows marked with the number 3.

It is also necessary to stress the following peculiarity seen in figure 3. The gap between the last occupied level and the nearest empty level strongly depends on  $B^{-1}$ . It is large at  $B^{-1} \leq 3$ , but shows pronounced minima at  $B^{-1} = 4, 7, 11, 14, 18, 21, \dots$ . All integer  $B^{-1}$  must correspond to the minima in the SdH conductivity (Ando *et al* 1982). However, when a particular gap is small the corresponding minimum will be smeared due to the finite temperature and the finite level width. Hence it may disappear from the experimental patterns. It follows from the data of Stormer *et al* (1983) on SdH oscillations for 2D holes (see figure 2 in their paper) that the first six oscillations follow one another regularly with the period in  $B^{-1}$  consistent with the value of  $n$ . However, for larger  $B^{-1}$  the mean period increases by a factor of about 2.5. It is very tempting to attribute this fact to the quasiperiodic change in the gap seen in figure 3 (there is no problem with the point  $B^{-1} = 4$ , since  $E_1^+$  is highly sensitive to the value of  $\delta$ ). However, to check the correctness of this hypothesis much more detailed experimental data are needed.

### 3. Magnetic susceptibility

The properties of the MS in a 3D semiconductor with a ring of extrema (the wurtzite lattice) were investigated by Boiko and Rashba (1960). It was shown that the MS has a singularity when the chemical potential  $\mu = 0$ , and the oscillatory part of the MS must show beats caused by existence of two close Fermi surfaces. These were soon discovered in crystals with the cubic zincblende lattice (Whitsett 1965, Roth *et al* 1967). It is natural to expect a non-trivial behaviour of the MS also to occur in 2D systems with a similar spectrum. However, when comparing the properties of 3D EG with those of 2D EG, it is important that in the first case  $\mu \approx \text{constant}$  follows from  $n = \text{constant}$  in the whole quasiclassical region while in the second case at  $n = \text{constant}$ ,  $\mu$  changes abruptly with the steps about  $\hbar\omega$  ( $T = 0$ ). This fact excludes the beats in dHvA and SdH oscillations for 2D EG (Vinter and Overhauser 1980), but the beats in the gap discussed above may be considered to be their relics.

Let us now calculate the MS  $\chi(B)$ . We shall do this for  $T = 0$  and consider the effect of finite  $T$  only qualitatively. One has to distinguish between the MS at  $\mu = \text{constant}$ ,  $\chi^{(\mu)}$ , and that at  $n = \text{constant}$ ,  $\chi^{(n)}$ . The direct calculation of  $\chi^{(n)}$  at arbitrary values of  $n$  and  $B$  is highly intricate due to the cumbersome form of  $\mu = \mu(n, B)$  for the energy spectrum (4). However, it seems plausible that the condition  $n = \text{constant}$  is the more

adequate for a variety of real experimental situations. Hence we shall start by deriving a general expression that connects  $\chi^{(n)}$  and  $\chi^{(\mu)}$  for a 2D EG.

It is useful to introduce a new quantum number  $N$  which includes both  $s$  and the index of the branch (+ or -), increases with energy ( $E_{N+1} > E_N$ ) and equals unity ( $N = 1$ ) for the ground state. Then the thermodynamic potential  $\Omega$  and the total energy  $E$  are

$$\Omega(\mu, B) = n_L \sum_{N'}' (E_{N'} - \mu) \quad (8)$$

$$E(n, B) = n_L \sum_{N' \leq N} E_{N'} + [n - (N - 1)n_L] E_N. \quad (9)$$

$N$  is the partly filled level. The prime in  $\Sigma'$  indicates that  $E_{N'} < \mu$ . This condition is very important, because it ensures complete definition of the derivative  $(\partial\Omega/\partial B)_\mu$ , which has a finite discontinuity at  $\mu = E_N$  due to the  $n_L$ -fold degeneracy (per unit area) of the Landau levels. It follows from (8) and (9) that

$$E(n) = (\Omega(\mu) + nE_N)_{\mu=E_N}. \quad (10)$$

Here and below we omit the argument  $B$ . It follows from (10) that  $\chi^{(n)} = -B^{-1}(\partial E/\partial B)_n$  is given by

$$\begin{aligned} \chi^{(n)}(n) &= \chi^{(\mu)}(\mu)|_{\mu=E_N-0} - [(n - n_L(N - 1))/B] dE_N/dB \\ \chi^{(\mu)}(\mu) &= -B^{-1}(\partial\Omega/\partial B)_\mu. \end{aligned} \quad (11)$$

To calculate  $\chi^{(\mu)}$  it is convenient to transform (4), as usual, using the Poisson formula. Then, for  $\delta > 0$  and  $-\Delta < \mu < -\delta\hbar\omega$  (cf figure 2) we get

$$\Omega(\mu) = n_L \hbar \omega \left( \int_{x_1}^{x_2} \varepsilon^-(x) dx - \frac{\mu(x_2 - x_1)}{\hbar\omega} - 2 \operatorname{Re} \sum_{l=1}^{\infty} \frac{1}{2\pi i l} \int_{x_1}^{x_2} e^{2\pi i l x} \frac{d\varepsilon^-(x)}{dx} dx \right), \quad (12)$$

and for  $\mu > \delta\hbar\omega$

$$\begin{aligned} \Omega(\mu) &= n_L \hbar \omega \left[ \int_0^{x_1} \varepsilon^+(x) dx + \int_0^{x_2} \varepsilon^-(x) dx - \frac{\mu(x_1 + x_2)}{\hbar\omega} + \delta \right. \\ &\quad \left. - 2 \operatorname{Re} \sum_{l=1}^{\infty} \frac{1}{2\pi i l} \left( \int_0^{x_1} e^{2\pi i l x} \frac{d\varepsilon^+(x)}{dx} dx + \int_0^{x_2} e^{2\pi i l x} \frac{d\varepsilon^-(x)}{dx} dx \right) \right] \end{aligned} \quad (13)$$

where  $\varepsilon^+(x_1) = \varepsilon^-(x_2) = \mu/\hbar\omega$ . Everywhere in what follows  $x_1$  and  $x_2$  must be expressed in terms of  $\mu$  using these conditions. Expressions for  $\Omega$  at  $-\delta < \mu/\hbar\omega < \delta$  may be written analogously. The last terms in (12) and (13) are transformed using integration by parts.

In the limit of weak fields  $B$ , when  $\gamma^2 \gg 1$  then  $x_2 \gg 1$ , but for  $x_1$  we may have either  $x_1 \approx 1$  or  $x_1 \gg 1$ . The last inequality holds only when  $|\mu| \gg (\hbar\omega\Delta)^{1/2}$ . It is convenient to integrate the last integrals in (12) and (13) once more by parts, since only a non-integral term must be retained in them in the leading order (this corresponds to the expansion in  $x_1^{-1}$ ,  $x_2^{-1} \ll 1$ ). Then expanding (12) and (13) in  $B$  and retaining the terms up to  $B^2$ , we obtain

$$\begin{aligned} \Omega(\mu, B) &= \Omega_0(\mu) + (rB^2/2\pi) \{ -\delta^2[(\Delta + \mu)/\Delta]^{1/2} \theta(-\mu) - (\delta^2 - \delta + \tfrac{1}{6})\theta(\mu) \\ &\quad + \tfrac{1}{2}B_2(x_1)(\Delta + \mu)^{1/2}/[\Delta^{1/2} - (\Delta + \mu)^{1/2}] \\ &\quad + \tfrac{1}{2}B_2(x_2)(\Delta + \mu)^{1/2}/[\Delta^{1/2} + (\Delta + \mu)^{1/2}] \}, \end{aligned} \quad (14)$$

where  $r = e^2/mc^2$ . Here  $\theta(z)$  equals 1 or 0 for  $z > 0$  or  $z < 0$ , respectively. The function  $B_2(x)$  is the second Bernoulli polynomial, which is equal to  $B_2(x) = x^2 - x + \frac{1}{6}$  at  $0 \leq x < 1$  and is periodic in  $x$  modulo 1.

When  $|\mu|$  is small,  $|\mu| < (\hbar\omega\Delta)^{1/2}$ , the third term in  $\Omega$  is large and is not described by (14). It gains its value from the region  $x_1 \sim 1$  and has the order of magnitude  $\Omega_1 \sim r\gamma B^2$ ,  $\gamma \gg 1$ .

From (14) we get that  $\chi^{(\mu)}$  is given by

$$\begin{aligned} \chi^{(\mu)} = (r/\pi) \{ & \delta^2 [(\Delta + \mu)/\Delta]^{1/2} \theta(-\mu) + (\delta^2 - \delta + \frac{1}{6}) \theta(\mu) \\ & - \frac{1}{2} B_2(x_1) (\Delta + \mu)^{1/2} / |\Delta^{1/2} - (\Delta + \mu)^{1/2}| \\ & - \frac{1}{2} B_2(x_2) (\Delta + \mu)^{1/2} / [\Delta^{1/2} + (\Delta + \mu)^{1/2}] \} \\ & + (n_L/B^2) (\mu + \Delta)^{1/2} \{ |\Delta^{1/2} - (\Delta + \mu)^{1/2}| B_1(x_1) \\ & + [\Delta^{1/2} + (\Delta + \mu)^{1/2}] B_1(x_2) \}. \end{aligned} \quad (15)$$

Here  $B_1(x)$  is the first Bernoulli polynomial, which is equal to  $B_1(x) = x - \frac{1}{2}$  at  $0 \leq x < 1$ , is periodic in  $x$  modulo 1 and is discontinuous at integer values of  $x$  (it has steps equal to  $-1$ ).

The terms in (15) including  $\theta(-\mu)$  and  $\theta(\mu)$  describe the monotonic part of  $\chi^{(\mu)}$ , while the other terms describe the oscillatory part. The final term (i.e. that proportional to  $(n_L/B^2)$ ) is of special importance, since it dominates at small  $B$  and introduces sawtooth oscillations typical of 2D EG (Seitz 1940) due to the discontinuous behaviour of  $B_1(x)$ . The magnitude of the steps in  $\chi^{(\mu)}$  is

$$\chi_\Delta^{(\mu)} = (n_L/B^2) (\mu + \Delta)^{1/2} |\Delta^{1/2} \pm (\Delta + \mu)^{1/2}| \sim (r/\hbar\omega) \max\{|\mu|, \Delta\} \gg r. \quad (16)$$

Oscillations may be observed only when  $T < \hbar\omega \sim \Delta/\gamma^2$ .

The gigantic diamagnetism  $\chi \sim -r\gamma^2$  arising from  $\Omega_1$  can be observed in a wider temperature range  $T < (\hbar\omega\Delta)^{1/2} \sim \Delta/\gamma$ . However, it arises only when  $\mu \approx 0$ , i.e.  $n \approx n_{cr}$ . At higher temperatures only the first two terms in (15) survive.

The second case, when the MS may be calculated, corresponds to strong fields  $B$ , when only a few levels are occupied, since  $E(n, B)$  includes a small number of terms. All the parameters of Hamiltonian (4) can be found in this region from the dependence on  $B$  of  $\chi^{(n)}$  or  $\chi^{(\mu)}$ .

The magnitude of steps  $\chi_\Delta$  in  $\chi$  can be easily determined at arbitrary  $n$  and  $B$ , e.g. using (9). The formulae have different forms in the three cases considered in § 2.

*Case 1.* The  $N$ th level becomes totally occupied and the filling of the  $(N + 1)$ th level begins:

$$\chi_\Delta^{(n)} = (n_L/B^2) N(E_{N+1} - E_N). \quad (17)$$

$\chi_\Delta^{(n)}$  diminishes when the gap  $E_{N+1} - E_N$  becomes small.

*Case 2.* The  $N$ th and  $(N + 1)$ th levels intersect (at  $B = B_{cr}$ ) with decreasing  $B$ :

$$\chi_\Delta^{(n)} = \{[n - n_L(N - 1)]/B_{cr}\}[(dE_N/dB)_+ - (dE_N/dB)_-]. \quad (18)$$

The subscripts  $+$  and  $-$  indicate that the derivative must be taken at the points  $B_{cr} + 0$  and  $B_{cr} - 0$ , respectively.

*Case 3.* The two levels that intersect are again the  $N$ th and  $(N + 1)$ th:

$$\chi_\Delta^{(n)} = \{[(N + 1)n_L - n]/B_{cr}\}[(dE_N/dB)_+ - (dE_N/dB)_-]. \quad (19)$$

When  $N \gg 1$ , expressions (18) and (19) take values smaller than that taken by (17), by a factor of about  $(\Delta/E_N)^{1/2}$ .

The analog of (17) for the case when a level  $E_N$  crosses the Fermi energy under the condition  $\mu = \text{constant}$  has the form

$$\chi_{\Delta}^{(u)} = -(n_L/B) dE_N/dB. \quad (20)$$

This expression is in agreement with the magnitude of steps following from (15).

Equations (17)–(20), together with the behaviour of  $\chi$  in strong fields and the peculiarities of all the oscillatory effects, connected with the level intersection (§ 2), provide us with a new tool for determining all the parameters of the Hamiltonian in the magnetic field:  $m$ ,  $\alpha$  and  $g$ .

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