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Excitations of modulated crystals near the commensurate-incommensurate transition

J. B. Sokoloff
Physics Department, Northeastern University, Boston, Massachusetts 02115
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The discommensuration (i.e., domain wall) lattice which appears when a modulated crystal (e.g., a crystal containing a charge or spin-density wave, etc.) undergoes a commensurate-incommensurate transition can introduce many closely spaced narrow gaps in the commensurate-state phonon and electron band structures. The locations of these narrow band gaps and the conditions under which they occur and are observable is discussed. Application to various incommensurate systems, including doped polyacetylene, is also discussed. In the case of doped polyacetylene, this band and gap structure may play an important role in the occurrence of a metal-insulation transition.

I. INTRODUCTION

During the past few years a good deal of effort has been devoted to the study of phase transitions in crystals which possess a modulation potential incommensurate with the crystal lattice (e.g., crystals containing charge[1] or spin-density waves,[2] mercury chain compounds,[3] etc.). In particular, much attention has been paid to the transition between the state in which the modulation is incommensurate and the state in which it is commensurate with the lattice.[4] There has not been much work, however, on the behavior of the elementary excitations of such systems in the vicinity of the commensurate-incommensurate transition. Away from the transition, however, the excitations are well understood.[5–10] Aubry showed that a one-dimensional tight-binding model with a sinusoidal modulation potential commensurate with the crystal lattice has a metal-insulator transition for modulation strength equal to the bandwidth.[5] In the insulation regime the wave functions are exponentially localized, whereas in the metallic regime, the states are extended and the band structure is Cantor-set-like (i.e., the bands are broken up by a hierarchy of band gaps, most of which are negligibly small[6,7]). For the modulation potential strength small compared to the bandwidth, almost all gaps are negligibly small, and thus, we would expect the system to behave as a normal metal. For potential strength just smaller than the bandwidth (the point at which the metal-insulator transition occurs), we expect the bands to be almost completely fragmented.[6] Unfortunately, for most samples, the modulation is relatively weak compared to the bandwidth, and hence, the unusual band structure due to incommensurability is simply never observable in most real experimental systems. Rather, the band structure is not much different in the incommensurate phase from that observed in the commensurate phase.

It should be remembered, however, that Aubry's model assumes a purely sinusoidal modulation potential, whereas when the system is nearly commensurate, the modulation is never sinusoidal. Rather, it consists of an array of domain walls or discommensurations, separated by large regions in which the lattice and modulation potential are commensurate.[10–12] The domain-wall lattice has a periodicity given by the difference between commensurate- and incommensurate-state wave vectors. Since such a potential has many Fourier components, it could perhaps produce the same multigapped spectrum, as occurs in the Aubry model for potential strength comparable to the bandwidth, but for much weaker potentials.

In this article a model for such a nearly commensurate system is studied. For an incommensurate state close to the $\frac{1}{2}$ registry, a series of very narrow bands appear in the commensurate-state gap when the system undergoes a commensurate-incommensurate transition. For all other registries, a structure consisting of very narrow bands separated by narrow gaps will appear at the commensurate-state band edges. For the $\frac{1}{3}$ and higher-order registries, this structure will only appear if the modulation strength is comparable in magnitude to the bandwidth. In this article, the conditions under which such effects appear will be discussed. These effects were already discussed for a sinusoidal modulation in Refs. 6 an 7.

II. LOCALIZATION OF THE PHONON AND ELECTRON SPECTRA OF THE FRENKEL-KONTOROVA MODEL DUE TO THE DISCOMMENSURATION LATTICE

Our model is the much studied Frenkel-Kontorova model (which consists of a chain of harmonically interacting atoms in a sinusoidal external potential).[10] The eigenvalue equation for the phonons in this

model is

$$\omega^2 u_n = \alpha(2u_n - u_{n-1} - u_{n+1}) + \lambda(\cos Q\bar{x}_n)u_n \ , \qquad (1)$$

where $\bar{x}_n$ is the atomic equilibrium position in the ground state, u_n is the displacement from equilibrium of the nth atom in the chain, α is the interatomic force constant, λ is the strength of the force constant due to the sinusoidal potential divided by the ionic mass and $Q = 2\pi/a$, where a is the period of the sinusoidal potential. Equation (1) could also be an approximate Schrödinger equation describing electrons, moving in the potential due to the modulation in the lattice. In this case, we identify u_n and ω^2 with the electron wave function and eigenvalue, respectively, and α and λ with the hopping matrix element and strength of the potential, respectively.

Aubry has argued using the KAM (Kolmagorov, Arnold, Moser) theorem that when the mean interatomic spacing b is incommensurate with a and the sinusoidal potential in the Frankel-Kontorova model[10] is sufficiently weak, $\bar{x}_n$ is of the form

$$\bar{x}_n = nb + \phi + g(nb + \phi) \ , \qquad (2)$$

where ϕ is an arbitrary phase and $g(x)$ is an analytic periodic function of period a whose form can depend only on b and the strength of the sinusoidal potential. This result implies the existence of a continuously degenerate ground state (i.e., we go from one ground state to the next by changing ϕ) and of a zero-frequency sliding mode.[13] If we substitute Eq. (2) into Eq. (1), we obtain a Schrödinger difference equation for a particle on a lattice in a potential of period a. We may always write b as $b = b_0 + \Delta b$, where b_0 is chosen so that b_0/a is of the form l/m, where l and m are integers chosen so that l/m closely approximates b/a. Then Eq. (1) becomes

$$\omega^2 u_n = \alpha(2u_n - u_{n-1} - u_{n+1}) + \lambda \cos Q[nb_0 + y + g(nb_0 + y)]u_n \ , \qquad (3)$$

where $y = n\Delta b + \phi$. Clearly, by appropriate choice of b_0, we may make Δb arbitrarily small, and hence make y a slowly varying function of n. Treating y as independent of n to lowest approximation, Eq. (3) may be diagonalized to obtain eigenvalues which we denote by $\omega_\alpha(k,y)$ where α is a band index and k is the wave vector. Following Ref. 6(b) we may use these "classical" trajectories to generate a quasiclassical treatment of the incommensurate problem, provided the bands found by diagonalizing Eq. (3) become independent of the phase y in the limit as l and m because infinite (i.e., as l/m better approximates b/a). We may find the equilibrium ionic $\bar{x}_n$ by solving the difference equation for the equilibrium configuration numerically by the methods of Ref. 14. For sufficiently weak sinusoidal potential in the Frenkel-Kontorova model there exist high-symmetry minimum-energy equilibrium configurations, separated by maximum-energy configurations, as a function of the phase variable ϕ.[14] The location of regions of allowed energy bands have been determined for values of the phase corresponding to maximum and minimum atomic configurations, using the continued fraction method outlined in Ref. 6. The results are shown in Figs. 1 and 2. We see that as b/a is approximated by higher-and-higher-order rational numbers, the energy spectrum becomes more and more independent of phase for $\lambda/x < 2.1$; for $\lambda/x \geq 2.1$ the reverse is true. Following the arguments of Ref. 6(c) we may argue that this result implies that the eigenfunction u_n is an analytic function of n for $\lambda/\alpha < 2.1$. For $\lambda/\alpha \geq 2.1$ the states are probably localized. Although we cannot rule out the possibility that there exists a small range of potential strengths over which there are both localized and extended states separated by a mobility edge, there is no evidence for its existence.

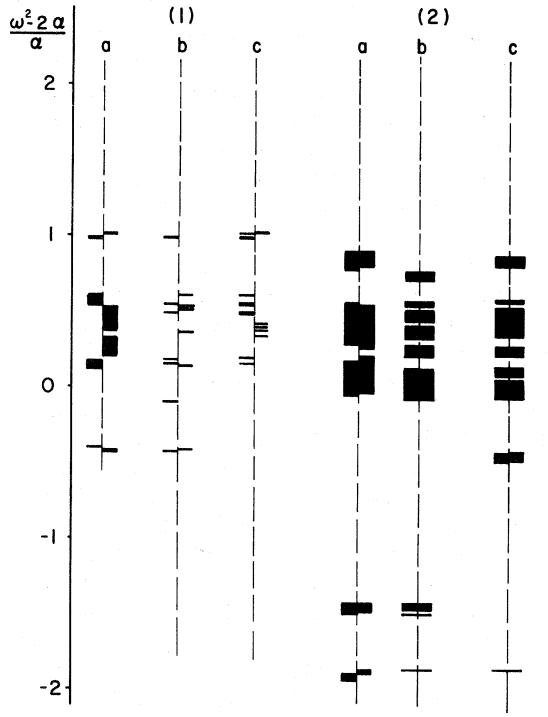

FIG. 1. Band structure from Eq. (3) (shaded areas are regions of allowed energy) for $Q =$ (a) $\frac{3}{10}$, (b) $\frac{10}{33}$, and (c) $\frac{33}{109} \times 2\pi/a$, which are successive approximations to

$$Q = (2\pi/a)\{1 + 1/[3 + 1/(3 + \cdots)]\}$$

for (1) $\lambda/\alpha = 2.1$, (2) $\lambda/\alpha = 1.5$ The band structure is given for the two values of the phase variable y which give maximum- and minimum-energy lattice configurations. The two sides of each dotted line represent different values of y.

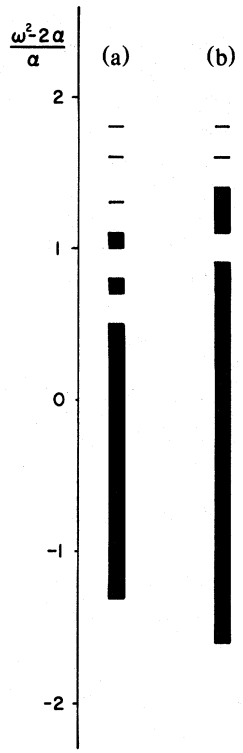

FIG. 2. Band structure from Eq. (3) for $Q=(2\pi/a)\frac{20}{21}$, which approximates an incommensurate state which has wave vector close to the fundamental registry (i.e., $Q=2\pi/a$) for (a) $\lambda/\alpha=0.6169$, (b) $\lambda/\alpha=0.3948$.

III. BAND STRUCTURE FOR A SYSTEM WHICH IS CLOSE TO THE FUNDAMENTAL REGISTRY

Let us now consider the band structure which occurs when $\lambda/\alpha<2.1$ (i.e., in the extended state regime). We will first study the case of a modulation whose period is nearly equal to that of the lattice, which is easier to visualize than high-order registry cases. Furthermore, as we shall see, near the top and bottom of the band the continuum approximation may be used, and the equations of motion in the continuum approximation may be solved exactly.

When Eq. (1) is taken to be the equation of motion for phonons in the Frenkel-Kontorova model, λ must have the value $\lambda=(2\pi/a)^2V_0$, where V_0 is the strength of the sinusoidal potential in the Frenkel-Kontorova model.[10] This is precisely the value for which, in the continuum approximation [i.e., when the difference operator in Eq. (1) replaced by a second-order differential operator[10]] Eq. (1) possesses only two phonon bands.[15] Thus, near the bottom of the phonon spectrum, where the continuum approximation should be valid, there can be only one gap in the spectrum. Higher in the spectrum where the continuum approximation is no longer valid, there should be the familiar multigapped spectrum.[6] To examine this, Eq. (1) was diagonalized for several high-order commensurate systems. The equilibrium positions $\bar{x}_n$ were determined by solving the equilibrium difference equations numerically.[14] The allowed bands of Eq. (1) were then found numerically using the continued-fraction method of Ref. 6. The results are illustrated in Fig. 2. For the vicinity of the fundamental registry (i.e., b nearly equal to a) near the top of the spectrum, we may again use a continuum approximation in order to obtain analytical results. Near the top of the band we may write $u_n=(-1)^n v_n$, where v_n is a slowly varying function of n. Since u_n is a analytic function of n, as argued earlier, we may write

$$v_{n+1}+v_{n-1}=2\cos\left(\frac{1}{i}\frac{d}{dn}\right)v_n\simeq 2\left(1-\frac{1}{2}\frac{d^2}{dn^2}+\cdots\right)v_n$$

for states near the top of the band (at which point $u_{n\pm1}\approx -u_n$). Substituting this result in Eq. (1), we obtain the following Schrödinger equation

$$-\frac{d^2}{dn^2}v_n+V(n)v_n=(\epsilon-\lambda)v_n \ , \tag{4}$$

where $\epsilon=\lambda+2x-\omega^2$ and $V(n)$ is the negative of the potential term in Eq. (1) (i.e., $-\lambda\cos Q\bar{x}_n$). In this case, the potential maximum occurs inside the domain walls instead of in the region between them. For such a case, the bands may be found using the method of Ashcroft and Mermin, which determines the energy bands for a periodic array of potential barriers.[16] When the domain walls are far apart, it is easily shown that $V(n)$ is given in the continuum approximation by[10]

$$V(n)=-\lambda\left(1-\frac{2}{\cosh^2[(\lambda/\alpha)n]^{1/2}}\right) \ . \tag{5}$$

According to Ashcroft and Mermin[16]

$$\cos(KL/b+\delta)=|t|\cos kL \ , \tag{6}$$

where $K=(\epsilon/\alpha)^{1/2}$, L is the separation between centers of adjacent domain walls, k is the wave vector of the band states, t is the transmission amplitude, and δ the phase of t. According to Landau and Lifshitz,[17]

$$|t|^2\approx\frac{(\pi KW)^2}{\cosh^2\frac{1}{2}\pi\sqrt{7}} \tag{7}$$

for this potential near the top of the band where K is small, and $W=\sqrt{\alpha/\lambda}$ is the width of a domain wall. Combining Eqs. (6) and (7), we find that the allowed

energy bands occur for

$$\frac{[(2n+1)\frac{1}{2}\pi-\delta]b}{L+AW} \leq k \leq \frac{[(2n+1)\frac{1}{2}\pi-\delta]b}{L-AW} \quad , \quad (8)$$

where

$$A=\frac{\pi}{\cosh\frac{1}{2}\pi\sqrt{7}} \approx 0.09844 \quad .$$

Clearly, as $\epsilon \to 0$, and the transmission coefficient goes to zero, the phase of the Eq. (8) must reduce to $\frac{1}{2}\pi$, so that the allowed energy bands occur at the energy levels for a particle trapped between two infinite energy barriers, i.e., there exist very narrow bands centered at energies

$$\epsilon=\alpha n^2\pi^2 b^2/L^2 \quad . \quad (9)$$

For example, for $2H$-$TaSe_2$ (Refs. 18 and 19) at 100°, the domain-wall spacing has been observed to be about 100 lattice constants, which gives energy levels of the order of $E \sim n^2 10^{-3}\alpha$. (We have chosen $2H$-$TaSe_2$ only as an illustration of typical domain spacing. Our results, of course, do not apply to $TaSe_2$ because it has a two-dimensional modulation.) For the electronic case, the potential strength is usually not equal to one of the particular values for which the transmission coefficient is unity,[17] and hence there should exist a similar gap structure at the bottom of the band as well. Of course, Eq. (9) is only valid when ϵ is much less than the potential strength.

IV. SPECTRUM NEAR HIGHER-ORDER REGISTRIES

In many systems containing incommensurate modulations, we are not interested in the vicinity of the fundamental registry (i.e., $b \sim a$). Rather we are interested in the vicinity of a higher-order registry, i.e., $b/a = l/m$, where l and m are small integers (such as 1, 2, 3, etc.) To study such cases we use the quasiclassical methods of Ref. 6. Such a study begins with the "classical trajectories," which are found by studying the energy-level structure as a function of the phase variable y in Eq. (3). The "classical" trajectories for the case of a sinusoidal potential [i.e., $\bar{x}_n = nb$ in Eq. (1)] of wave vector $Q=(2\pi/a)(l/m)+q$ with $q \ll Q$ are found by treating qnb as a constant phase in Eq. (1) and diagonalizing Eq. (1) for the resulting commensurate problem. The resulting secular determinent is easily shown to be of the form

$$\frac{\pi}{\alpha}[\omega^2-\omega_\alpha^0(k)^2]+2(\lambda/2\alpha)^m(1-\cos mqbn)=0 \quad , \quad (10)$$

where $\omega_\alpha^0(k)$ are the band frequencies for $n=0$.[6] The solutions of this equation for ω^2 give the "classical" trajectories. For small λ/α, this turns out to also be a good estimate of the "classical" trajectories for the domain case discussed earlier. The gaps introduced by the fact that the system is incommensurate are found by solving the quantum-mechanical problem which results from replacing the difference operators in Eq. (1) by differential operators, i.e., $u_{n\pm1} \sim \cos[(qb/i)\,d/dy]u(y)$, where the position variable is $y=qnb$ and $u(y)=u_n$. The resulting infinite-order Schrödinger equation has qb playing the role of $\hbar$, and hence, if qb is small we may apply the WKB approximation. In Ref. 6(b) it is shown that if we do this, formally diagonalize the resulting commensurate problem and then requantize the WKB approximation equations, we find that we must solve the effective Schrödinger equation

$$\omega_\alpha^2\left(\frac{qb}{i}\frac{d}{dy},y\right)u(y)=\omega^2 u(y) \quad ,$$

where $\omega_\alpha^2(k,y)$ is one of the solutions to Eq. (10). This is simply the conventional way of treating the problem of electrons in a solid in the presence of an external field as discussed in most textbooks.[20] The quasiclassical methods used by Zilberman[21] may now be applied directly to this effective Schrödinger equation. We find that the gap structure comes about primarily because there exist localized classical trajectories which get broadened into narrow bands and because gaps are introduced in those extended trajectories which lie close in energy to the local trajectories.[21] On the other hand, in most incommensurate systems studied to date $\lambda/\alpha \approx 10^{-2}$, and hence, we see from Eq. (10) that the position dependence of the "classical" trajectories will be negligibly small for $m \geq 3$. In such a case there will be practically no localized trajectories, and hence, almost no observable gap structure introduced when the commensurate-incommensurate transition occurs. For $\lambda/\alpha \approx 1$, the structure will be observed but the system is more likely to be locked into the commensurate phase. For example, for the fundamental registry case (i.e., $m=1$) if $\lambda/\alpha=1$, the system locks into registry for $|b-a|/a \leq 0.2$.[10] For the case in which there is a discommensuration-lattice potential rather than a sinusoidal potential, we may use the the methods of Refs. 14 and 6 in the way described in Sec. II of this article to find the allowed energy bands. The resulting band structure shows no gap structure for $m \geq 3$ if λ/α is as small as 10^{-2}. The band structure for $\lambda/\alpha \approx 1$ is illustrated in Fig. 3 for the $m=3$ case.

The $m=2$ case, however, is special because the classical trajectories are given by

$$\omega^2=2\alpha \pm (4\alpha\cos^2\tfrac{1}{2}kb+\lambda^2\cos^2 qbn)^{1/2} \quad (11)$$

for the sinusoidal potential case with $Q=(\pi/b)+q$ ($q \ll Q$). Thus, no matter how small we make

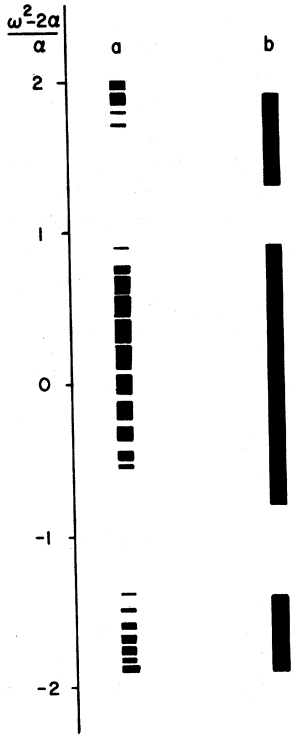

FIG. 3. Band structure from Eq. (3) calculated for $Q=(2\pi/a)\frac{10}{31}$, which approximates an incommensurate state close to the $\frac{1}{3}$ registry for (a) $\lambda/\alpha=0.9638$, (b) $\lambda/\alpha=0.3448$.

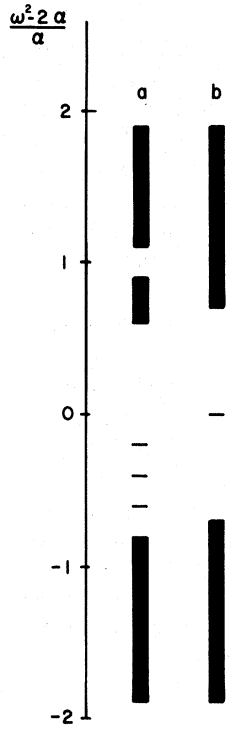

FIG. 4. Band structure for $\lambda/\alpha=0.61685$ for $Q=(2\pi/a)\frac{15}{31}$ which approximates an incommensurate state close to the $\frac{1}{2}$ registry for (a) the domain model and (b) the sinusoidal potential for comparison.

λ/α, the gap in the spectrum will vary from 0 to λ as we move through the crystal. This implies the existence of localized "classical" trajectories, no matter how small the potential strength λ. For ω^2 near the center of the gap, the trajectories are approximately elliptical. To see this, expand Eq. (11) about the point $k=\pi/2b$ and $qbn=\frac{1}{2}\pi$. Using the quasiclassical method outlined in Ref. 6(b), it can be shown that the quantization condition for a closed orbit "classical" trajectory is that the area of the orbit be equal to $2\pi qnb$, where n is a positive integer. The reason that we get n rather than $n+\frac{1}{2}$ is that the quasiclassical wave function is proportional to[6(b)]

$$e^{-k(x)b}\exp\frac{i}{qb}\left(\int^x k(x')\,dx\right), \tag{12}$$

where $x=qnb$ and $k(x)$ is the result of solving Eq. (11) for k. When x is analytically continued about the classical turning points to obtain the connection formulas,[22] the exponential prefactor in Eq. (12) does not give the phase factor as occurs in the usual WKB method, for which the prefactor $\sim[k(x)]^{-1/2}$. Thus, following the methods of Ref. 22, we get n instead of $n+\frac{1}{2}$. The area of the elliptical trajectory is found to be $\pi(\omega^2-2\alpha)^2/2\alpha\lambda$ and hence the quantization method given above gives

$$\omega^2=2\alpha\pm(2\alpha\lambda qbn)^{1/2} \tag{13}$$

for $n=0$, the expansion of Eq. (11) about the point $k=\pi/2b$, $qbn=\pi/2$, is certainly valid. For $n=1$, it will be valid only if $(2\alpha\lambda qb)^{1/2}$ is much less than the gap energy, which is equal to λ. Thus, it is clear that this method will only be valid for qb very small. This method, of course, neglects the broadening of the levels into bands, and hence, will only be valid if the bands are extremely narrow. For the discommensuration-potential case we must again resort to the numerical methods of Refs. 6 and 14 outlined in Sec. II. Some resulting band structures are shown in Fig. 4. We see that the band structure is no longer symmetric about the center of the gap and there are more levels inside the gap than for the pure sinusoidal potential case.

V. CONCLUSIONS

It has been shown that when a one-dimensional crystal with a modulation undergoes a commensurate-incommensurate transition, there will appear structure consisting of narrow bands separated by narrow gaps. This structure will occur only at the

commensurate-state band edges for all except the $\frac{1}{2}$ registry, for which narrow bands will also appear at the center of the commensurate-state gap. Most modulated systems studied to date have a commensurate phase which is of higher order than the $\frac{1}{2}$ registry and have modulation potentials that are too weak for this structure to be observable. Stronger modulation potentials will occur, however, for ionic conductors such a hollandite,[23] for example. The fundamental and $\frac{1}{2}$ registries were shown to exhibit observable structure, even for weak modulation potentials. Examples of materials with a fundamental and $\frac{1}{2}$ registry, respectively, are thiourea and $(NH_4)_2BeF_4$.[24] Another important example of an incommensurate system which is close to the $\frac{1}{2}$ registry is doped polyacetylane,[25] which is believed to possess a soliton lattice.[26,27] The single-soliton case possesses an electronic bound state at the center of the band gap.[25] According to the results of the present article, there might be several very narrow bands appearing inside the gap of polyacetyline when it is doped and hence possesses a soliton lattice,[26,27] although the present model is not precisely applicable to this material. This band structure can have important effects on the optical and transport properties of this material. The narrow-band states inside the commensurate-state gap should become localized states if the ordered-to-chaotic state transition predicted by Bak and Pokrovsky occurs.[26] The reason for this is that the bands that occur inside the commensurate-state gap are essentially due to states localized in the domain walls. When the domain walls form an ordered array, these states get broadened into narrow bands. In the chaotic phase the domain walls have random spacing, which will tend to localize these states. This localization transition could play a role in the observed metal-insulation transition.[28] Such phenomena will be discussed in more detail in future publications.

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