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Magnetic subband structure of Bloch electrons in a two-dimensional lattice under magnetic modulation

Paula Fekete and Godfrey Gumbs†

Department of Physics and Astronomy, Hunter College of the City University of New York,
695 Park Avenue, New York, NY 10021, USA

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Abstract. This paper presents an analytical and numerical investigation of the energy spectrum of two-dimensional Bloch electrons subject to a periodic potential of square and hexagonal symmetry and a perpendicular sine-modulated magnetic field, applying the tight-binding model. The energy spectrum is found using an effective Hamiltonian obtained by employing the Peierls substitution in the ground-state energy band function. The resulting Schrödinger equation is solved by applying a matrix method. The energy spectrum found exhibits recursive properties similar to those discussed by Hofstadter for the case of a uniform perpendicular magnetic field. It is the objective of this paper to show that this technique can be extended successfully in the presence of a modulated magnetic field of arbitrary strength. We successfully demonstrate a Hofstadter-type spectrum in the presence of both a uniform and a modulated magnetic field.

1. Introduction

The energy spectrum of an electron system under the influence of both a periodic potential and a magnetic field has been intensively studied in the last three decades. Recent studies of the effects of a periodic magnetic field have attracted renewed theoretical interest in the field [1–8]. With the development of submicron lithography and nano-fabrication techniques it became possible to create crystals in which experimental indications of the Hofstadter spectrum can be found, demonstrating the validity of the underlying physics [9–13].

Theoretical solution of the problem of the energy spectrum for electron systems has been addressed in two fundamentally different ways. The tight-binding and the nearly-free-electron methods are known to represent opposite approaches to the calculation of the electronic band structure in crystals. The tight-binding method, applicable in the limit of weak magnetic fields, is a semiclassical method, which starts from electron states localized in real space at different lattice sites and introduces a single-band effective Hamiltonian by the application of the Peierls's substitution [14–17]. The nearly-free-electron method, on the other hand, is a quantum mechanical approach that is suitable for strong magnetic fields [18–23]. It starts from plane waves localized in reciprocal space and uses free-electron Landau eigenstates as a basis and the periodic lattice potential as a perturbation. It is well known that there is a strong resemblance between the energy spectrum of 2D tight-binding electrons subject to a uniform perpendicular magnetic field, and that of electrons in Landau states interacting with a 2D periodic potential. The inclusion of harmonic functions, corresponding to the excited

† Also at: The Graduate School and University Center of the City University of New York, 33 West 42 Street, New York, NY 10036, USA

states in the matrix elements of the potential, is equivalent to tight-binding models with more nearest-neighbour interactions [21]. In the study of 2D electrons in a magnetic field the use of the tight-binding model has provided significant insight. Most of the knowledge that we have concerning the spectrum and density of states in magnetic fields derives from the analysis of simple square or hexagonal tight-binding Hamiltonians [24–27]. These analyses suggest that a recursion is present in the energy spectrum. Increased attention has been given lately to the study of the spectrum in the case where there is an anisotropy of the hopping integrals. An asymmetry in the hopping strength can lead to a closing of the gaps [28].

Recently there has been extensive study of electronic properties of 2D electron systems under nonuniform magnetic fields. However, these studies focused on the effects of magnetic modulation on free electrons while the problem of calculating the effect of magnetic modulation on Bloch electrons remains far less explored.

This paper studies the electronic properties of a two-dimensional (2D) electron system (ES) under the influence of both a periodic potential and a perpendicular one-dimensional (1D) sine-modulated (SM) magnetic field. The solution to this problem is sought by following the semiclassical method applicable in the low-magnetic-field regime. The method was first introduced by Peierls [27] and consists of replacing the Hamiltonian by the tight-binding electron energy operator $E(\mathbf{k})$ with the Bloch index \mathbf{k} replaced by the operator $(\mathbf{p} - e\mathbf{A})/\hbar$. The resulting Schrödinger equation is a finite-difference equation whose eigenvalues can be computed for arbitrary wavenumbers by using a matrix approach. Following the calculations of Gumbs, Miesse, and Huang [29] the Harper equation is modified by adding an additional flux-dependent phase factor due to the SM magnetic field.

Recently [29], we chose a parameter for the modulating field which was not applicable and thereby obtained some inaccurate numerical results. Here, we now show how a modulating magnetic field leads to energy band structure that is different from the Hofstadter's spectrum and demonstrate how the self-similarity appearing in the Hofstadter's spectrum breaks down. Also, we present results for anisotropic hopping on the lattice in the presence of a modulating magnetic field [30]. Our method [29] can predict the energy spectrum of 2D electrons in a square lattice under magnetic modulation, since the method has no theoretical flaws. For rational values of a/b (where a is the lattice constant, while b is the period of the modulating field) not equal to one, the model works when the amplitude of the modulating magnetic field is small compared with the uniform component. This paper underlines the importance of paying the required attention to even the smallest detail in the process of applying simplifications to mathematical relations when working in a certain theoretical model, as the conclusions drawn depend on the outcome of the calculations. It should however, be pointed out that the newly conducted calculations do not in any way confirm the applicability of the assumption that the Hofstadter-type spectrum disappears under the conditions of study.

2. General formulation of the problem

2.1. Square lattice

Consider a two-dimensional square lattice with the corresponding periodic potential in the x - y plane and the magnetic field in the z -direction. The magnetic field is expressed as $\mathbf{B} = [B_0 + B_1(x)]\hat{z}$ where B_0 is the magnitude of the uniform component and B_1 is the magnitude of the modulation field. Although other types of modulation are also possible, this paper discusses the sine-modulated field

$$\mathbf{B} = \left[B_0 + B_1 \sin\left(\frac{2\pi x}{b}\right) \right] \hat{z} \quad (1)$$

parallel to the z -axis, where b is a constant. The corresponding vector potential is $\mathbf{A} = (0, A_y(x), 0)$ in the Landau gauge with

$$A_y(x) = B_0 x - \frac{B_1 b}{2\pi} \cos\left(\frac{2\pi x}{b}\right). \quad (2)$$

Assuming a tight-binding dispersion $\varepsilon(k)$, Hofstadter [24] obtained the Schrödinger equation

$$\varepsilon(k) = 2t_x \cos(k_x a) + 2t_y \cos(k_y a) \quad (3)$$

where t_x and t_y are the tunnelling bandwidths in the x - and y -directions and a is the lattice constant. Make the Peierls substitution

$$k_x \rightarrow \hat{p}_x/\hbar \quad k_y \rightarrow (\hat{p}_y + eA_y(x))/\hbar. \quad (4)$$

This yields the effective Hamiltonian

$$\hat{\mathcal{H}}(\mathbf{p}) = t_x \left\{ e^{ia\hat{p}_x/\hbar} + e^{-ia\hat{p}_x/\hbar} \right\} + t_y \left\{ e^{iae\hat{A}_y(x)/\hbar} e^{ia\hat{p}_y/\hbar} + e^{-iae\hat{A}_y(x)/\hbar} e^{-ia\hat{p}_y/\hbar} \right\}. \quad (5)$$

Using the property of translational operators in the plane $e^{-i\mathbf{R}\cdot\hat{\mathbf{p}}/\hbar}|\mathbf{r}\rangle = |\mathbf{r} + \mathbf{R}\rangle$ along with the Schrödinger equation $\hat{\mathcal{H}}(\mathbf{p})|\mathbf{r}\rangle = E|\mathbf{r}\rangle$ leads us to the eigenvalue equation for the ground-state energy of an electron in the 2D square lattice:

$$t_x [\phi_k(x-a, y) + \phi_k(x+a, y)] + t_y \left[e^{iae\hat{A}_y(x)/\hbar} \phi_k(x, y-a) + e^{-iae\hat{A}_y(x)/\hbar} \phi_k(x, y+a) \right] = E\phi_k(x, y). \quad (6)$$

We now set $x = ma$, $y = na$ where m and n are integers. In the Landau gauge the variable y is cyclic and can be separated in equation (6) using the following relation:

$$\phi_k(ma, na) = \exp(ik_y na) g_k(m).$$

As a consequence, the Schrödinger equation becomes

$$t_x [g_k(m-1) + g_k(m+1)] + 2t_y \cos\left(\frac{ae\hat{A}_y(x)}{\hbar} - k_y a\right) g_k(m) = E g_k(m). \quad (7)$$

Equation (7) can be rewritten to give the modified Harper equation in matrix form for the square lattice with a SM magnetic field as

$$\begin{pmatrix} g_k(m+1) \\ g_k(m) \end{pmatrix} = \begin{pmatrix} \tilde{\varepsilon} - \Delta_m(k_y, \alpha, \beta) & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} g_k(m) \\ g_k(m-1) \end{pmatrix} \quad (8)$$

with

$$\Delta_m(k_y, \alpha, \beta) \equiv 2\eta \cos\left(2\pi m\alpha - \frac{\alpha}{\beta} \gamma \cos(2\pi m\beta) - k_y a\right). \quad (9)$$

Here, we have introduced the following notation:

$$\alpha = a^2 B_0 / (h/e) \quad \beta = a/b \quad \gamma = B_1 / B_0 \\ \eta = t_y / t_x \quad \tilde{\varepsilon} = E / t_x.$$

Thus the effect of magnetic modulation can be studied without any condition imposed on the modulating field. The modified Harper equation (8) in the presence of magnetic modulation has an additional term proportional to γ which is the ratio of the amplitude of the magnetic modulation to the uniform magnetic field when the amplitude of the modulating field is much less than the constant external magnetic field.

Assume that $\alpha = p/q$ where p and q are integers and let m take all integer values from 1 to q in equation (8) to generate a system of q equations. These q equations only repeat themselves if $\beta = 1$ which means by equation (1) that there is no effect from modulation since

we set $x = ma$. If a and b are not commensurate, i.e., β is irrational, there is no periodicity in the x -direction. Consequently, there is no fixed relation between α and the number of split subbands in a Bloch band. If β is irrational, there is no fractal band structure. However, when $\beta = r/s$, where r and s are integers, the equations for $g_k(m)$ will be unchanged under the replacement $m \rightarrow m + sq$. Therefore, the period in the x -direction will be $sq a$ instead of qa when there is no modulation, and there will be sq subbands split from a Bloch band for $\alpha = p/q$.

We now use the Bloch condition for the electron wavefunction and take

$$g_k(0) = e^{-ik_x sq a} g_k(sq) \quad g_k(sq + 1) = e^{ik_x sq a} g_k(1). \quad (10)$$

Thus, we have transformed a two-dimensional problem into a one-dimensional one. Moreover, it will be sufficient to only solve the problem in the first magnetic Brillouin zone and within a unit cell. Since Harper's equation is periodically repeated after sq cycles, equations (8) and (10) together give the following eigenvalue equation:

$$\tilde{\epsilon} \begin{pmatrix} g_k(1) \\ g_k(2) \\ \dots \\ g_k(sq - 1) \\ g_k(sq) \end{pmatrix} = \mathbf{A}(\mathbf{k}, \alpha, \beta) \begin{pmatrix} g_k(1) \\ g_k(2) \\ \dots \\ g_k(sq - 1) \\ g_k(sq) \end{pmatrix} \quad (11)$$

where the matrix to be diagonalized is

$$\mathbf{A}(\mathbf{k}, \alpha, \beta) = \begin{pmatrix} \Delta_1 & 1 & 0 & 0 & 0 & \dots & 0 & 0 & e^{-ik_x sq a} \\ 1 & \Delta_2 & 1 & 0 & 0 & \dots & 0 & 0 & 0 \\ 0 & 1 & \Delta_3 & 1 & 0 & \dots & 0 & 0 & 0 \\ 0 & 0 & 1 & \Delta_4 & 1 & \dots & 0 & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & 0 & 0 & \dots & \Delta_{sq-2} & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & \dots & 1 & \Delta_{sq-1} & 1 \\ e^{ik_x sq a} & 0 & 0 & 0 & 0 & \dots & 0 & 1 & \Delta_{sq} \end{pmatrix}. \quad (12)$$

From the matrix equation (11), we deduce the following conclusions:

- (a) For $\gamma = 0$, there is no modulating magnetic field, and the matrix reduces to the one obtained by Hofstadter [24].
- (b) For a chosen value of $\beta = a/b$, $\cos(2\pi m\beta)$ in the second term of equation (9) vanishes for certain values of m , leading to the cancelling of the modulating component. These values are $m = (2L + 1)/(4\beta)$, where L is an integer. This means that for certain choices of the modulation period, there is no contribution due to the modulating field to the matrix elements in equation (12).
- (c) For the wave-vector replacement $k_x \rightarrow -k_x$, there is a corresponding change $\mathbf{A}(\mathbf{k}, \alpha, \beta) \rightarrow \mathbf{A}^*(\mathbf{k}, \alpha, \beta)$. Therefore, the energy eigenvalues are not altered by this change in the wave vector.
- (d) When $\gamma = 0$ and $k_y \rightarrow -k_y$, $m \rightarrow -m$, the matrix $\mathbf{A}(\mathbf{k}, \alpha, \beta)$ in equation (12) is unchanged. Therefore, the energy eigenvalues remain the same under this transformation. This is not true for $\gamma \neq 0$.

- (e) When $k_x \rightarrow k_x + 2\pi j/(sqa)$, for any integer j , we obtain the same matrix $\mathbf{A}(\mathbf{k}, \alpha, \beta)$ in equation (12). This implies that all of the eigenvalues have period $2\pi/(sqa)$ in k_x -space for any fixed value of sqa . This is true for both cases with $\gamma = 0$ and with $\gamma \neq 0$.
- (f) If $k_y \rightarrow k_y \pm 2\pi j/a$, for any integer j , all eigenvalues remain the same. This means that the energy spectrum in k_y -space has period $2\pi/a$. Moreover, for $k_y \rightarrow k_y + 2\pi j\alpha/a$, equation (12) will be unchanged when $m \rightarrow m + j$, for $\gamma = 0$. However for $\gamma \neq 0$, this matrix invariance is only true if $j\beta$ is an integer.
- (g) When $\gamma = 0$, clearly for $k_y = 0$, the transformations $\alpha \rightarrow \ell - \alpha$ and $\alpha \rightarrow -\alpha$ in equation (12) are equivalent to the change $m \rightarrow -m$. As a result, all of the energy eigenvalues remain the same under this transformation for an infinite 2D square lattice. However, this symmetry is broken for $\gamma \neq 0$.

Figure 1 shows the rational magnetic flux versus the energy eigenvalues for a square lattice in the presence of a uniform as well as a modulating magnetic field. In this figure, the hopping is isotropic with the hopping energies in the x - and y -directions given by $t_x = t_y = 1$. In figure 2 the amplitude of the magnetic modulation is the same as for figure 1 with $\gamma = B_1/B_0 = 2.0$, but here $\eta = t_y/t_x = \frac{1}{2}$. In both plots, the wave vector \mathbf{k} and the ratio of the period of the lattice to that of the modulating magnetic field $\beta = a/b$ are the same and are given in the figure captions. Clearly the magnetic modulation breaks the reflection symmetry of the eigenvalue spectrum about $\alpha = 0.5$. Also, these calculations show that the gaps in the energy spectrum are altered considerably. We have also computed the eigenvalues for finite wave vector to examine the effect on the energy spectrum. These results, not shown here, indicate that the energy eigenvalues depend on both k_x and k_y . In the presence of a strong modulating magnetic field, figures 1 and 2 show that there are states for $\alpha = 0.5$ for negative energies but there are none for positive energies. This means that a strong modulating magnetic field causes the eigenvalue spectrum to be noticeably asymmetric about the zero of energy. Also, the energy spectra in figures 1 and 2 for $\alpha = 0.5$ are broadened when compared with the results in reference [30].

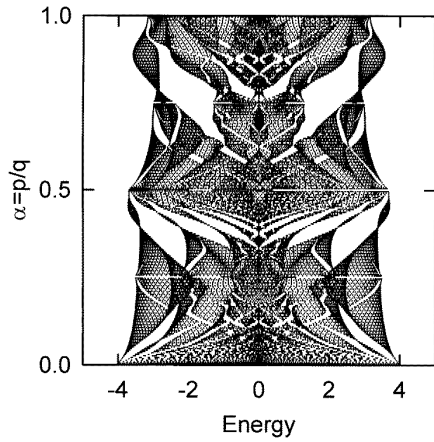


Figure 1. The energy E/t_x of a square lattice in a perpendicular magnetic field as a function of the rational flux quantum $\alpha = p/q$. The parameters used in the calculation are $\eta = t_y/t_x = 1$, $\beta = a/b = \frac{1}{4}$, and $\gamma = B_1/B_0 = 2.0$. The wave vector is chosen with $k_x = 0, k_y = 0$.

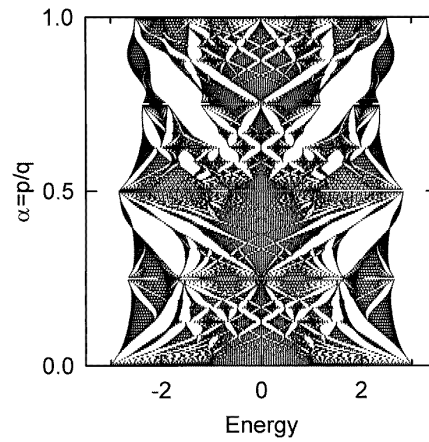


Figure 2. The same as figure 1, except that the hopping on the lattice is anisotropic such that $\eta = t_y/t_x = \frac{1}{2}$.

2.2. Hexagonal lattice

We now turn to the calculation of the energy eigenvalues for the hexagonal lattice in the presence of magnetic modulation as well as a uniform perpendicular magnetic field. We recently obtained the eigenvalue spectrum for the hexagonal lattice in a uniform external perpendicular magnetic field [31]. We now extend these calculations to analyse the effect due to a modulating magnetic field and compare the results with the square lattice presented above.

For a 2D lattice with hexagonal symmetry, it can be shown that in the absence of an external magnetic field, the lowest energy band with anisotropic nearest-neighbour overlap is given by [31]

$$E = 2E_0 \left\{ t_0 \cos(k_x a) + t_+ \cos((k_x + k_y \sqrt{3})a/2) + t_- \cos((k_x - k_y \sqrt{3})a/2) \right\} \quad (13)$$

where a is the lattice constant and the atom at the origin has nearest neighbours $(\pm a, 0)$ and $(\pm a/2, \pm \sqrt{3}a/2)$, and $\mathbf{k} = (k_x, k_y)$ is the wave vector of an electron. In this notation, t_0 is the nearest-neighbour overlap in the x -direction and t_{\pm} are the nearest-neighbour overlap integrals along the symmetry directions which make angles of $\pi/3$ and $2\pi/3$ with this direction. E_0 is an energy scale related to the bandwidth. We now use the Peierls substitution to construct the Hamiltonian in the presence of a constant external magnetic field B_0 and a sinusoidal magnetic field of amplitude B_1 in the x -direction. After a straightforward calculation [31], we obtain the following matrix which must be diagonalized to determine the energy eigenvalues:

$$\begin{pmatrix} 0 & \delta_1 & \frac{t_0}{t_+} & 0 & 0 & \dots & 0 & \frac{t_0}{t_+} e^{-ik_x sqa} & \delta_1^* e^{-ik_x sqa} \\ \delta_2^* & 0 & \delta_2 & \frac{t_0}{t_+} & 0 & \dots & 0 & 0 & \frac{t_0}{t_+} e^{-ik_x sqa} \\ \frac{t_0}{t_+} & \delta_3^* & 0 & \delta_3 & \frac{t_0}{t_+} & \dots & 0 & 0 & 0 \\ 0 & \frac{t_0}{t_+} & \delta_4^* & 0 & \delta_4 & \dots & 0 & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & 0 & 0 & \dots & 0 & \delta_{sq-2} & \frac{t_0}{t_+} \\ \frac{t_0}{t_+} e^{ik_x sqa} & 0 & 0 & 0 & 0 & \dots & \delta_{sq-1}^* & 0 & \delta_{sq-1} \\ \delta_{sq} e^{ik_x sqa} & \frac{t_0}{t_+} e^{ik_x sqa} & 0 & 0 & 0 & \dots & \frac{t_0}{t_+} & \delta_{sq}^* & 0 \end{pmatrix} \quad (14)$$

where

$$\delta_m \equiv (t_-/t_+) e^{i\mu_m} + e^{-i\mu_m} \quad (15)$$

with

$$\mu_m \equiv 2\pi m(p/q) - k_y a - \frac{\alpha}{\beta} \gamma \cos(2\pi m\beta). \quad (16)$$

Here, we assumed that the flux through a unit cell of the hexagonal lattice is $\alpha = p/q$ and the ratio of the period of the lattice to the period of modulation is $\beta = r/s$ where p, q, r , and s are integers. We have also defined γ in the same way as we did for the square lattice.

Figures 3 and 4 show plots of the rational magnetic flux versus the energy eigenvalues for a hexagonal lattice in the presence of a uniform and modulating magnetic field. The ratio of the amplitude of the magnetic modulation to the constant external field is chosen as $\gamma = B_1/B_0 = 2.0$. The wave vector \mathbf{k} and the ratio of the period of the lattice to that of the

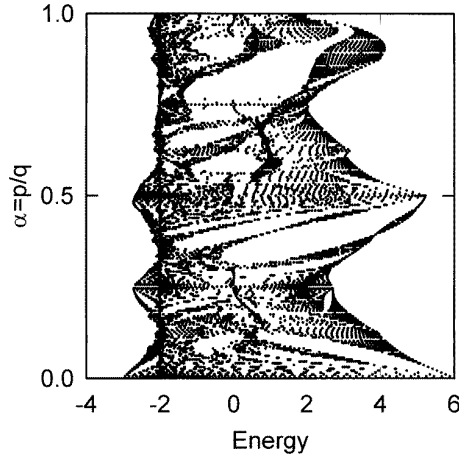


Figure 3. The energy E/t_+ of a hexagonal lattice in a perpendicular magnetic field as a function of the rational flux quantum $\alpha = p/q$. The parameters used in the calculation are $t_0 = t_-/t_+ = 1$, $\beta = a/b = \frac{1}{4}$, and $\gamma = B_1/B_0 = 2.0$. The wave vector is chosen with $k_x = 0, k_y = 0$.

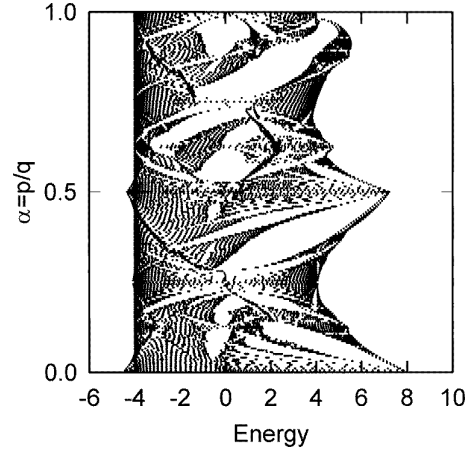


Figure 4. The same as figure 3, except that $t_0 = 2$ and $t_-/t_+ = 1$.

modulating magnetic field $\beta = a/b$ are the same in the two figures. In figure 3, the coefficients in equation (13) are chosen as $t_0 = t_- = t_+ = 1$, whereas in figure 4, we have $t_0 = 2$ and $t_- = t_+ = 1$. These results should be compared with the plots for the energy spectrum of a hexagonal lattice when only a uniform external magnetic field is applied [31].

3. Summary and concluding remarks

In this paper, we have presented a general formulation for determining the energy spectrum of two-dimensional Bloch electrons subject to a periodic potential of square and hexagonal symmetry and a uniform as well as a sine-modulated magnetic field. We apply the tight-binding model for the lowest energy band and obtain the energy spectrum in the presence of a magnetic field by using an effective Hamiltonian obtained by employing the Peierls substitution. The method is valid when the modulation magnetic field is of arbitrary strength. The resulting Schrödinger equation is solved numerically by applying a matrix method when the magnetic flux through a unit cell of the lattice per flux quantum is a rational fraction and when the ratio of the period of modulation to the period of the lattice is also rational. The calculated energy spectrum exhibits recursive properties similar to those discussed by Hofstadter for the case of a uniform perpendicular magnetic field. Our results show that the presence of modulation affects the symmetry properties of the energy spectrum.

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