Crossing rule for a \mathcal{PT} -symmetric two-level time-periodic system

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For a two-level system in a time-periodic field we show that in the non-Hermitian \mathcal{PT} case the level crossing is of two quasistationary states that have the *same* dynamical symmetry property. At the field's parameters where the two levels which have the same dynamical symmetry cross, the corresponding quasienergy states coalesce and a self-orthogonal state is obtained. This situation is very different from the Hermitian case where a crossing of two quasienergy levels happens only when the corresponding two quasistationary states have *different* dynamical symmetry properties and, unlike the situation in the non-Hermitian case, the spectrum remains complete also when the two levels cross.

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I. INTRODUCTION

The question of what conditions two energy levels cross as the potential parameters are varied was addressed many years ago by von Neumann [1], Landau and Lifshitz [3], Teller [2], and Longuet-Higgins [4]. All these studies were carried out for time-independent systems and within the standard (Hermitian) formalism of quantum mechanics. Here we address the dynamics of a driven two-level system, which has been a subject of interest for many years in different fields of physics (see, for example, Refs. [5-9]). The motivation to study the conditions for crossings of two quasistationary solutions in a driven two-level system is twofold. The first motivation is to determine the hidden symmetry in the Hermitian two-level system driven by a time-periodic field which enables two quasienergy levels to cross as the laser field parameters are varied. Ivanov, Corkum, and Dietrich derived the condition for crossings of two quasienergy levels when the laser frequency is much larger than the transition frequency, which is defined as the excitation energy, $\hbar\omega_{21}$, divided by the Planck constant \hbar [10]. More recently, Šindelka has shown that when the two quasi-energy levels cross the assumption that the laser field can be treated classically when the laser intensity is large (many photons interact with the quantum two level system) does not hold and the light-matter interaction should be studied within the formalism of quantum electrodynamics although high field intensity is used [11]. We show here that the "hidden symmetry" in the Hermitian case is the dynamical symmetry. The two quasienergy levels that cross in the studies of Ivanov and his co-workers and of Šindelka are two different (nondegenerate) quasienergy eigenstates of the dynamical symmetry operator (which is defined below). The second motivation is to study the crossing of two quasienergy levels in the non-Hermitian case. The fact that, in a non-Hermitian time-independent Hamiltonian which consists of a linear combination of two Hermitian noncommutative operators, one can always find a complex parameter where two eigenstates cross was proved a long time ago [12]. Most recently, it was shown by Lefebvre and his co-workers [13] that two complex quasienergies which are associated with the photoinduced

dissociative resonances of H_2^+ are crossed. The crossing of the quasienergy (Floquet) resonances has a dramatic effect on the ability to control the dynamics of H_2^+ in moderate laser fields [13]. We wish to show here that in the case of the non-Hermitian time-periodic Hamiltonian the quasienergies that cross when the laser intensity is increased are two degenerate eigenstates of the dynamical symmetry operator which are defined below. This situation is very different from the situation in a Hermitian time-periodic Hamiltonian where the two quasienergy levels which cross are two nondegenerate eigenstates of the dynamical symmetry operator. Without loss of generality of our study of the dynamics of non-Hermitian driven two-level systems, here we have chosen to study the dynamics of a very special non-Hermitian-driven system where the time-dependent Hamiltonian has a \mathcal{PT} symmetry and therefore the quasienergy levels should be real as long as the field strength parameter gets a sufficiently small value. The \mathcal{PT} properties of a *time-independent* Hamiltonian are the focus of interest in different fields of physics [14-19].

II. THE DYNAMICAL SYMMETRY (DS) OPERATOR FOR DRIVEN TWO-LEVEL SYSTEMS

The time-periodic Hamiltonian of a driven two-level system in our study is given below (in atomic units where $\hbar = 1$) as

$$\mathbf{H}(t) = \mathbf{H}_0 + \mathcal{E}_0 \mathbf{V}(t)$$

= $\frac{\omega_{21}}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + \mathcal{E}_0 \cos(\omega t) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$ (1)

where ω_{21} is the transition frequency in the two-level system and \mathcal{E}_0 is the maximum field amplitude multiplied by the dipole transition matrix element. In the Hermitian case, \mathcal{E}_0 gets real values only. In the non-Hermitian case, \mathcal{E}_0 gets complex values (i.e., the dipole matrix element is a complex number). As we show below, a non-Hermitian \mathcal{PT} symmetry time-periodic Hamiltonian is obtained when \mathcal{E}_0 gets imaginary values only, i.e., $\operatorname{Re}\mathcal{E}_0 = 0$ whereas $\operatorname{Im}\mathcal{E}_0 \neq 0$. The time-independent \mathcal{PT} symmetric two-level Hamiltonian, which can be obtained from Eq. (1) by letting the frequency go to zero, is proportional

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to the two-level Hamiltonian studied in Ref. [20] where the proportional factor is *i*. Therefore, instead of solving

$$\mathbf{H}(t)a(t) = i\frac{\partial a(t)}{\partial t}$$
(2)

using our model Hamiltonian, we should multiply the above time-dependent Schrödinger equation by the imaginary number *i* such that $i\mathbf{H}(t) = \mathbf{H}_{\text{Ref. [20]}}(t)$ and solve the diffusion like equation

$$\mathbf{H}_{\text{Ref. [20]}}(t)a(t) = -\frac{\partial a(t)}{\partial t}.$$
(3)

The quasistationary solutions of the Hermitian and of the non-Hermitian time-dependent Schrödinger equations are given by

$$H_F a_i(t) = \epsilon_i a_i(t), \quad i = 1, 2,$$

$$H_F \equiv -i \frac{d}{dt} \mathbf{I} + \mathbf{H}(t),$$
(4)

where

$$a_i(t) = a_i \left(t + \frac{2\pi}{\omega} \right). \tag{5}$$

The terminology of quasienergy comes from the fact that if $0 \le \epsilon_i \le \omega$ is an eigenvalue of the Floquet operator H_F then $\epsilon_i + \omega N$; $N = 0, \pm 1, \pm 2, \ldots \pm \infty$ is an eigenvalue of H_F which is associated with the eigenvector $a_i(t)e^{i\omega Nt}$.

Therefore, the complete quasienergy spectrum of the Floquet operator H_F is given by

$$H_F b_{i,N}(t) = (\epsilon_i + \omega N) b_{i,N}(t)$$

{*i* = 1,2; *N* = ±1,±2,...,±∞}, (6)

where $b_{i,N}(t) = a_i(t)e^{i\omega Nt}$. The spectrum of the Floquet operator, $\epsilon_i + \omega N$ (i = 1, 2 in our case), splits between different Brillouin zones where |N| = 0, 1, 2, ... stands for the |N|th Brillouin zone. For example, N = 0 is the first Brillouin zone with quasienergies embedded within the energy interval of $[0, \pm \omega]$ (here $\hbar = 1$) where the second Brillouin zone is defined for the quasienergies within the energy interval $[\pm \omega, \pm 2\omega]$, and so on.

The DS has profound spectroscopic implications in Hermitian quantum mechanics, as shown by Alon and his co-workers [21]. In our case the second-order DS operator is defined as

$$\hat{P}_2 = \left\{ \tilde{\mathbf{H}}_0; \ t \to t + \frac{\pi}{\omega} \right\},\tag{7}$$

where

$$\tilde{\mathbf{H}}_0 = \frac{2}{\omega_{21}} \mathbf{H}_0 = \begin{pmatrix} 1 & 0\\ 0 & -1 \end{pmatrix}, \tag{8}$$

such that

$$\hat{P}_2 H_F(t) \hat{P}_2 = \tilde{\mathbf{H}}_0 H_F \left(t + \frac{\pi}{\omega} \right) \tilde{\mathbf{H}}_0 = H_F(t)$$
(9)

and therefore

$$[\hat{P}_2 H_F, H_F \hat{P}_2] = 0 \tag{10}$$

at any given time *t*.

From Eq. (10) we obtain that the eigenstates of the Floquet operator (regardless if it is a Hermitian operator or not), $b_{i,N}(t)$,

are eigenstates of the dynamical symmetry operator \hat{P}_2 . We can divide $b_{i,N}(t)$ [and therefore $a_i(t)$] into two groups of degenerate eigenstates of the dynamical symmetry operator,

$$\hat{P}_{2}a_{i}^{(+)}(t) = +a_{i}^{(+)}(t), \quad i = 1, 2,$$

$$a_{i}^{(+)}(t) = \begin{pmatrix} \sum_{m=-\infty}^{+\infty} c_{m,i}^{(+)} e^{i2m\omega t} \\ \sum_{m=-\infty}^{+\infty} d_{m,i}^{(+)} e^{i(2m+1)\omega t} \end{pmatrix},$$
(11)

where $a_i^{(+)}(t)$ are associated with the eigenvalues $-\hbar\omega \leq \epsilon_i \leq 0$ of the Floquet operator (here $\hbar = 1$) and

$$\hat{P}_{2}a_{i}^{(-)}(t) = -a_{i}^{(-)}(t), \quad i = 1, 2,$$

$$a_{i}^{(-)}(t) = \begin{pmatrix} \sum_{m=-\infty}^{+\infty} c_{m,i}^{(-)} e^{i(2m+1)\omega t} \\ \sum_{m=-\infty}^{+\infty} d_{m,i}^{(-)} e^{i2m\omega t} \end{pmatrix},$$
(12)

where the corresponding eigenvalues of $a_i^{(-)}(t)$ are $0 \le \epsilon_i \le \hbar \omega$ (here $\hbar = 1$). The Floquet eigenstates are orthonormal and, therefore, $\sum_m [c_{m,i}^{(\pm)}]^2 + \sum_m [d_{m,i}^{(\pm)}]^2 = 1$. Note that in the normalization condition given in the preceding equation we take the squares of the linear coefficients and not the absolute values because the coefficients might get complex values only when the Hamiltonian is non-Hermitian. For the definition of the "inner product" in non-Hermitian time-dependent and time-independent cases, see Ref. [22].

III. THE CROSSINGS OF DEGENERATE AND NONDEGENERATE EIGENSTATES OF THE DYNAMICAL SYMMETRY OPERATOR

Following the "noncrossing rule" as described by Teller within the Hermitian formalism of quantum mechanics, it is unlikely for two degenerate states of the dynamical symmetry operator to cross as a potential parameter \mathcal{E}_0 is varied. Two cases are studied here. The first case is when $\mathcal{E}_0 = \text{Re}\mathcal{E}_0$ and the time-periodic Hamiltonian is Hermitian. The second case is when $\mathcal{E}_0 = i\text{Im}\mathcal{E}_0$ and the time-periodic Hamiltonian is non-Hermitian. This non-Hermitian time-periodic Hamiltonian has the \mathcal{PT} symmetry which is defined here as

$$\hat{PT} = \{ \mathbf{H}_0; \ i \to -i; \ t \to -t \}, \tag{13}$$

such that

$$\hat{PTH}_F(t)\hat{PT} = \mathbf{H}_0[H_F(t)]^*\mathbf{H}_0 = H_F(t).$$
 (14)

Using perturbation theory for the Floquet operator where V(t) is the perturbation and $i|\mathcal{E}_0|$ is the perturbation strength parameter similar to the proof presented in Ref. [19], one can prove that the quasienergies of the \mathcal{PT} non-Hermitian Floquet operator get real values only as long as $|\mathcal{E}_0| < |\mathcal{E}_0|_{BP}$ where two quasienergy levels with the same dynamical symmetry cross, and where BP stands for a branch point. This branch point is commonly referred to as an exceptional point (EP) in the spectrum of the Hamiltonian. In our case it is an EP in the quasienergy spectrum of the non-Hermitian \mathcal{PT} Hamiltonian of a two-level system in time-periodic field. The proof that at some parameter region the spectrum of the (2n + 1) rule stated by Wigner [23], which in our case implies that the

(2n + 1) order of corrections to the eigenvalues of the Floquet operator are given by

$$\epsilon_i^{(2n+1)} = \frac{\omega}{2\pi} \int_0^{2\pi/\omega} a_i^{(n)}(t) \mathbf{V}(t) a_i^{(n)}(t) \, dt.$$
(15)

The zero-order Floquet operator is $-i\partial_t + \mathbf{H}_0$ and the perturbation strength parameter is \mathcal{E}_0 . The eigenvectors of the zero-order Floquet operator are given by

$$a_1^{(0)}(t;m) = e^{i\omega m t} \begin{pmatrix} 0\\1 \end{pmatrix},$$

$$a_2^{(0)}(t;m) = e^{i\omega m t} \begin{pmatrix} 1\\0 \end{pmatrix},$$
(16)

where $m = 0, \pm 1, \pm 2, ...$ Without loss of generality, we chose as the zero-order eigenvector $a_i^{(0)}(t; m = 0)$, where i = 1 (or another possibility is to choose i = 2). Since

$$\mathbf{V}(t)a_1^{(0)}(t;m=0) = \cos(\omega t)a_2^{(0)}(t;m=0),$$

$$\mathbf{V}(t)a_2^{(0)}(t;m=0) = \cos(\omega t)a_1^{(0)}(t;m=0),$$
(17)

where $a_1^{(0)}(t; m = 0) \times a_2^{(0)}(t; m = 0) = 0$, then the first-order correction to the quasienergy eigenvalue vanishes; i.e., $\epsilon_i^{(1)} = 0$ for i = 1 and i = 2. Using Eqs. (15)–(17), the first-order corrections to the exact eigenvectors obtained

$$a_1^{(1)}(t) = \frac{\cos(\omega t)}{\epsilon_1^{(0)} - \epsilon_2^{(0)}} a_2^{(0)}(t; m = 0),$$

$$a_2^{(1)}(t) = \frac{\cos(\omega t)}{\epsilon_2^{(0)} - \epsilon_1^{(0)}} a_1^{(0)}(t; m = 0),$$
(18)

and therefore, using Eq. (15), we get that $\epsilon_i^{(3)} = 0$ for i = 1and i = 2 while $\{\epsilon_i^{(2)}\}_{i=1,2} \neq 0$. Note that $\{\epsilon_i^{(2)}\}_{i=1,2}$ are real numbers, and so are all correction terms in general, $\{\epsilon_i^{(2)}\}_{i=1,2}$.

Using the standard expressions of nondegenerate perturbation theory for the *n*th corrections to the eigenvectors, one gets that all the odd-order corrections to the eigenvalues of the Floquet operator vanish and

$$\epsilon_i^{(2n+1)} = 0 \tag{19}$$

where i = 1,2 and consequently

$$\epsilon_i = \sum_{n=0}^{\infty} \mathcal{E}_0^{2n} \epsilon_i^{(2n)},\tag{20}$$

provided the perturbational series expansion is converged. The perturbational series expansion is converged when $|\mathcal{E}_0|$ is smaller than the radius of convergence, which by definition is equal to the absolute value of the branch point, $|\mathcal{E}_{BP}|$, which is closest to the origin at $\mathcal{E}_0 = 0$. Since in the non-Hermitian \mathcal{PT} -symmetry case

$$\mathcal{E}_0 = i |\mathcal{E}_0| \tag{21}$$

and $\mathcal{E}_0^{2n} = (-1)^n |\mathcal{E}_0|^{2n}$, then from Eq. (20) one can see that within the radius of convergence ϵ_1 and ϵ_2 get real values and the spectrum of the non-Hermitian \mathcal{PT} -symmetry time-periodic Floquet operator is real (at some parameter region defined above). Here our proof has been completed.



FIG. 1. (Color online) The quasienergy levels (a.u.) in two Brillouin zones as obtained from numerical calculations for the Hermitian-driven two-level system (\mathcal{E}_0 gets real values only) using 101 Floquet channels (i.e., $n = 0, \pm 1, \ldots, \pm 50$ in Eqs. (11) and (12)]; $\omega_{21} = 0.1$ and $\omega = 1$. The two quasienergy levels that cross are associated with two *nondegenerate* eigenstates of the dynamical symmetry operator \hat{P}_2 (red curves are the quasienergies of the degenerate states of \hat{P}_2 associated with the eigenvalue -1 (denoted by (-) in the plot), whereas the black curves are associated with the +1 eigenvalue (denoted by (+) in the plot). The crossings of the quasienergies are obtained at the transition from the first Brillouin zone to the second one, when the different zero-order Bessel function $J_0(\frac{2\mathcal{E}_0}{\omega}) = 0$ exactly as derived in Ref. [10].

The results presented in Fig. 1 clearly show that indeed in the Hermitian case, crossing takes place only between two quasienergies which have *different* dynamical symmetry (and localized at different Brillouin zones), whereas the results presented in Fig. 2 show that in the non-Hermitian case the two quasienergy levels which cross have the same dynamical symmetry (and localized at the same Brillouin zone). Since in the Hermitian case the crossing takes place between quasienergy levels from different Brillouin zones, the quasienergy at the crossing points should be at the edges of the Brillouin zones, $\epsilon_{\text{crossing}}^{\text{Hermitian}} = \omega N; \quad N = 0, \pm 1, \pm 2, \dots, \pm \infty.$ Since in the non-Hermitian case the crossings take place between quasienergy levels which are localized in the same Brillouin zone and since the trace of the Floquet operator is vanished at any given time, the level crossing for the \mathcal{PT} Floquet operator should be at the middle of the Brillouin zones, $\epsilon_{\text{crossing=BP}}^{\mathcal{PT}\text{-non-Hermitian}} = \omega(\frac{1}{2} + N); \ N = 0, \pm 1, \pm 2, \dots, \pm \infty.$

The results presented in Fig. 3 show that, as the two \mathcal{PT} quasienergy levels which are degenerate eigenstates of the dynamical symmetry operator \hat{P}_2 are sufficiently far from the crossing point, then

$$\epsilon_{1} \simeq \frac{\omega_{21}}{2} J_{0} \left(\frac{2i|\mathcal{E}_{0}|}{\omega} \right),$$

$$\epsilon_{2} \simeq -\frac{\omega_{21}}{2} J_{0} \left(\frac{2i|\mathcal{E}_{0}|}{\omega} \right) + \omega,$$
(22)

where J_0 are the zero-order Bessel functions. The failure of the analytical expressions for the two \mathcal{PT} quasienergy levels as a function of \mathcal{E}_0 to describe the behavior of the quasienergy



FIG. 2. (Color online) The complex quasienergy levels (a.u.) as a function of the Im \mathcal{E}_0 as obtained from numerical calculations for the non-Hermitian \mathcal{PT} -driven two-level system (\mathcal{E}_0 gets imaginary values only) using 101 Floquet channels [i.e., $n = 0, \pm 1, \ldots, \pm 50$ in Eqs. (11) and (12)]. The two quasienergy levels that cross are associated with two *degenerate* eigenstates of the dynamical symmetry operator \hat{P}_2 . [The red curves are the real quasienergies of the degenerate states of \hat{P}_2 associated with the eigenvalue -1 (denoted by (-) in the plot), whereas the black curves are associated with the +1 eigenvalue (denoted by (+) in the plot).] The (blue) curves are the imaginary parts of the quasienergy eigenvalues, showing that up to the crossing point the quasienergies are real although the Hamiltonian is non-Hermitian.

levels close to the crossing point results from the fact that, sufficiently close to the crossing point,

$$\epsilon_{1,2} = \epsilon_{\rm BP} \pm \alpha \sqrt{|\mathcal{E}_0| - \mathcal{E}_0|_{\rm BP}},\tag{23}$$

where the two normalized corresponding quasienergy eigenstates $[\psi_1 \equiv a_1^{(\pm)}(t) \text{ and } \psi_2 \equiv a_2^{(\pm)}(t)]$ collapse into the



FIG. 3. (Color online) The real part of the complex quasienergy levels (a.u.) in the first Brillouin zone as shown in Fig. 2 for the non-Hermitian \mathcal{PT} -driven two-level system which has the same dynamical symmetry. Up to the crossing point, the two quasienergies are real. Beyond the crossing point, they get complex values. [See the imaginary parts of the quasienergy eigenvalues in Fig. 2 (blue line).] The dashed lines are $\frac{\omega_{21}}{2} J_0(\frac{2|\mathcal{E}_0|i}{\omega})$ and $-\frac{\omega_{21}}{2} J_0(\frac{2|\mathcal{E}_0|i}{\omega}) + \omega$.



FIG. 4. The overlapping integral (using the standard Hermitian scalar product) of a linear combination of the two quasienergy eigenstates of the \mathcal{PT} -driven two-level model Hamiltonian which have the same dynamical symmetry property as a function of the imaginary part of \mathcal{E}_0 (a.u.). This plot shows that as the two quasienergy eigenvalues coalesce the corresponding quasienergy eigenstates also coalesce. (The phase factor $e^{i\pi/2} = i$ results from the different normalizations of the two quasienergy states [22].)

self-orthogonal eigenstate ψ_{BP} as $|\mathcal{E}_0| \rightarrow |\mathcal{E}_0|_{BP}$ for which $(\psi_{BP}|\psi_{BP}) = 0$:

$$\psi_{1,2} = \mathcal{N}_{1,2}[\psi_{\rm BP} \pm \chi \sqrt{|\mathcal{E}_0| - |\mathcal{E}_0|_{\rm BP}}],\tag{24}$$

where the normalization factors are related one to another by a phase factor such that $N_2 = iN_1$ (see Ref. [22]). The results presented in Fig. 4 clearly show that, as the two quasienergy eigenvalues coalesce, the corresponding quasienergy eigenstates also coalesce. The fact that the quasienergy eigenstates with the same dynamical symmetry coalesce implies a loss of one linearly independent eigenstate and thereby it gives birth to a self-orthogonal state at the crossing point.

IV. CONCLUDING REMARKS

The crossings between two quasienergy levels in the case that the driven two-level system is Hermitian results from the fact that those states are *not* degenerate states of the dynamical symmetry operator as defined in Eq. (5). At the crossing points which are located at the edges of the different Brillouin zones, the corresponding quasienergy eigenvectors are two different degenerate states. In the case where the laser frequency is larger than the frequency transition, our numerical results are in remarkable agreement with the analytical expressions for the quasienergies which where derived in Ref. [10].

In the non-Hermitian case (even for a non- \mathcal{PT} -symmetrydriven two-level system), crossings between degenerate states of the dynamical symmetry operator are obtained. Unlike the situation in the Hermitian case, there is only one crossing point of two quasienergy levels in each of the Brillouin zones. At the crossing point of the two quasienergy levels, the corresponding quasienergy eigenvectors coalesce as well and a self-orthogonal vector is obtained (see Fig. 4, where the norm of a linear combination of the two quasienergy vectors is vanished as the two corresponding quasienergy levels cross). For the \mathcal{PT} non-Hermitian time-periodic Hamiltonian, it is a point of interest that the analytical expressions derived for the quasienergy levels in the Hermitian case [10] also hold for the non-Hermitian case when the laser frequency is larger than the transition frequency between the two quasienergy levels as long as they get real values.

Last but not least, the non-Hermitian model Hamiltonian of driven two-level systems (not necessarily with \mathcal{PT} symmetry) describes physical situations where a bound state (or a resonance-metastable state) interacts with another resonance state as a laser field is turned on. An example is an atom in a combined dc and ac field. The dc field (or alternatively a low-frequency laser) turns the ground and the first excited bound states into resonances. The resonances are *complex* square integrable functions and are embedded in the generalized Hilbert space when one of the similarity transformations occurs as described in Ref. [22]. For non-Hermitian Hamiltonians rather than the usual scalar product one should use the so-called complex(c)-product [24], and complex expectation values (including dipole transition amplitudes) are obtained. For the physical interpretation of complex expectation values, see

Refs. [22,25]. In such a case the transition frequency ω_{21} and the dipole transition $d_{21} \equiv \epsilon_0/E_0$ in our model Hamiltonian get complex values. The imaginary part of the transition frequency, $-2\text{Im}\omega_{21}$, is the difference in the ionization rates of decay between the two resonance states. The duration of the laser pulse (introducing an ac field), which couples the two resonances, should be sufficiently long to justify the use of Floquet theory. Another example involves a laser field coupled between a ground bound state and an autoionization or Auger (resonance) states. Note, however, that one should look for specific atoms (or molecules) for which the non-Hermitian Hamiltonian has \mathcal{PT} symmetry. Another possibility is to associate our model Hamiltonian with optical wave guides. For example, our studies can be associated with the \mathcal{PT} -symmetry optical lattices suggested in Ref. [26] when a periodic index of refraction along the light propagation axis is introduced.

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