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Chaos In 2D Bohmian Trajectories of Commensurate Harmonics Oscillators

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ABSTRACT

Particle trajectories guided by the wave function are well-defined through Bohmian mechanics, which is a causal interpretation of quantum mechanics. Periodic and chaotic behaviours could be exhibited from the certain classical integrable systems that have been shown within this framework. In this study, we developed Mathematica programs to plot the Bohmian trajectories and Lyapunov exponents. These programs serve as computer experiments for numerical generation and illustration of the results. We show that the behaviours of commensurate two-dimensional harmonic oscillator systems are dependent on ratios of frequency.

1. Introduction

Standard quantum mechanics remains a probabilistic theory due to its unpredictable results in any measurement [1]. There has been extensive research regarding this fact to develop a deterministic quantum theory and one of the prominent ones is Bohmian mechanics.

The theory is named after David Bohm who rediscovered it after being abandoned by De Broglie in 1927 [2]. In the beginning, Pauli and other researchers criticized this theory [3] but nowadays, it has become more subjected to intense experimental and theoretical study. The Bohmian mechanics is mainly about a well-defined position with the wavefunction that guided its trajectory. The Bohmian trajectory clearly gives an intuitive idea and concepts which provide a causal connection between events in physical space time. Hence, this notion can become an alternative approach to solving problems in quantum mechanics. The study of quantum chaos is one of the problems that have been well investigated which was trying to understand the relationship between two phenomena in physics that are chaos and quantum theories. We noted that the periodic orbits, attractors, phase space maps and many other concepts of classical chaos have relied on the classical notion of trajectory. However, the situation is absolutely different for the microscopic system as the dissimilarities of fundamental implications are exists between standard quantum mechanics and

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classical mechanics. The concept of classical mechanics such as position and trajectory are not acceptable due to the fact of Heisenberg uncertainty principle that the position and momentum of each particle cannot be measured precisely at the same time. Moreover, the concept of physical systems state in standard quantum mechanics is also affected by the wave-particle duality. Meanwhile, wavefunction evolution must satisfy the Schrodinger equation in which the linearity of this evolution had made the wavefunction became less sensitive to the initial condition. All these factors cause the notion of chaotic trajectories not able to adopt directly in standard quantum mechanics. In an attempt to solve this problem, physicists had to find the criteria of quantum mechanics that can trace the existence of chaos in the quantum domain. There are several approaches discovered based on the statistical distribution of energy eigenvalue spacing and spatial correlations of wavefunction but unfortunately, they still cannot be compared directly.

Recently, the formulation of quantum mechanics based on Bohm's trajectories had attracted considerable interest from researchers. Several studies discussed chaos in Bohmian mechanics for numerous systems, e.g. cat map [4], the hydrogen atom in an oscillating electric field [5], two-dimensional harmonic oscillator [6] and kick rotor [7]. In Bohmian mechanics, chaos has been founded when the corresponding classical system is non-chaotic [8]. The trajectory of chaotic Bohmian may also appear even if there is no chaos occurring in standard quantum mechanics [9]. Besides that, unlike classical mechanics, Bohmian mechanics has an extra potential, namely quantum potential. In most quantum systems the quantum potential undergoes rapid fluctuations in space and time and contributes to chaos [10]. Moreover, some papers have shown that chaos in the Bohmian framework has been successfully demonstrated by the Lyapunov exponent which is a well-known chaos indicator in classical mechanics. This might be a powerful tool to visualize the correlation between classical chaos and Bohmian chaos. Guglielmo Iacomelli and Marco Pettini compared the stability differences between the classical regime and quantum regime in 1996 by applying the Lyapunov exponent [11]. Furthermore, there is also been reported that the Lyapunov exponent has to be demonstrated at least two dimensions of a system for chaos to occur in the Bohmian framework [12]. This indicated that nodal points which generated the vortices can be the one of chaos sources [13]. In this context, the relationship study between a quantum system and its classical counterpart has an advantage for Bohmian mechanics as we can make a quantitative comparison for both trajectories in this framework by using the Lyapunov exponent.

Therefore, the objective of this study was to investigate the chaotic behaviours of two-dimensional commensurate harmonic oscillators in the Bohmian mechanics framework by using the Lyapunov exponent. A particular concern is given to the change of rational frequency ratio and whether it influences the behaviour of this system.

2. Bohmian Mechanics Formulation

We have started with the Schrodinger equation to obtain the Bohmian equation of motion,

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V(t)\psi \tag{1}$$

Then we expressed the wavefunction in a polar form.

$$\psi(x,t) = R(x,t)\exp\left[\frac{i}{\hbar}S(x,t)\right] \tag{2}$$

with R and S are real functions. We substituted Eq. (2) into Eq. (1) to get a time evolution of R and S.

$$i\hbar \frac{d(Re^{\frac{iS}{\hbar}})}{dt} = \frac{\hbar^2}{2m}\nabla^2(Re^{\frac{iS}{\hbar}}) + V(x)(Re^{\frac{iS}{\hbar}}) \tag{3}$$

Hence we get a pair of couple equation.

$$\frac{dR}{dt} = \frac{1}{2m}(R\nabla^2 S + 2\nabla R \nabla S) \tag{4}$$

$$\frac{dS}{dt} = -\frac{(\nabla S)^2}{2m} + V(x) - \frac{\hbar^2 \nabla^2 R}{2mR} \tag{5}$$

Eq. (4) is referred to as the continuity equation where $R^2 = |\psi|^2$ is the probability distribution of position meanwhile Eq. (5) is similar in form of the Hamiltonian-Jacobi equation.

$$-\frac{\partial S}{\partial t} = \frac{(\nabla S_c)^2}{2m} + V \tag{6}$$

Nevertheless, there are two important differences. First, the term S in Eq. (5) represents the quantum state phase but in Hamilton's principal function, S_c is the relation $\nabla S_c = p(x,t)$ where p is the conjugate momenta in generalized coordinate in which both term clearly refer into two different phsyical concepts. However, if we assumed that $\nabla S = p(x,t)$, then we may respect the Eq. (5) as a quantum Hamilton-Jacobi equation for real quantum particles with well-defined trajectory. We called $\nabla S = p(x,t)$ as guidance condition where p is the particle's canonical momentum in Bohmian trajectory. Second, the additional term,

$$Q = \frac{\hbar^2 \nabla^2 R}{2mR} \tag{7}$$

is called "quantum potential" which is the only thing that makes Eq. (5) differently compared to the usual classical Hamiltonian-Jacobi equation. If we relate Q with force, similar to a classical force is attached with a classical potential energy, then we obtain,

$$F_Q = -\nabla Q \tag{8}$$

Here, F_Q is known as quantum force. Bohmian mechanics become more identical to Newtonian formulation from this expression, hence, the total force exerted on a quantum particle becomes,

$$F_t = -\nabla(V + Q) \tag{9}$$

Therefore, we defined firstly the velocity vector field as below to derive the guiding equation,

$$v = \frac{\nabla S}{m} \tag{10}$$

as we know $\nabla S = p(x,t)$. Then by substituting Eq. (2) into Eq. (10) we eventually obtained,

$$v(t) = \frac{i}{\hbar}\frac{\psi * \nabla\psi - \psi\nabla\psi *}{|\psi|^2} \tag{11}$$

3. Bohmian Trajectory of 2D Commensurate Harmonic Oscillator

The system that we chose in this study is the two-dimensional commensurate harmonic oscillator. It must have at least two degrees of freedom to form three coupled nonlinear autonomous differential equations. According to the Poincare Bendixcon theorem, these three such equations may generate chaos [14]. The Hamiltonian of a particle in this system is given by

$$H(x,y) = -\frac{1}{2}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + \frac{1}{2}(\omega_1 x^2 + \omega_2 y^2) \tag{12}$$

where, x and y are the position of the particle, $\omega_1$and ω_2 are the frequencies of the oscillator.

Considered the superposition of three eigenstates of this system as following,

$$\psi_{0,0} = \frac{\alpha}{\sqrt{\pi}} e^{\frac{1}{2}(\omega_1 x^2 + \omega_2 y^2)} e^{-\frac{i}{2}(\omega_1 + \omega_2)t}$$
$$\psi_{0,1} = \frac{2y\alpha}{\sqrt{\pi}} e^{\frac{1}{2}(\omega_1 x^2 + \omega_2 y^2)} e^{-\frac{i}{2}(\omega_1 + 3\omega_2)t}$$
$$\psi_{1,0} = \frac{2x\alpha}{\sqrt{\pi}} e^{\frac{1}{2}(\omega_1 x^2 + \omega_2 y^2)} e^{-\frac{i}{2}(3\omega_1 + \omega_2)t}$$

Here, $\alpha = (\omega_1\omega_2)^{\frac{1}{2}}$ and the corresponding eigenstate $\psi_{0,0}$ $\psi_{0,1}$ and $\psi_{1,0}$ refer to the ground state energy and the degenerate first excited states respectively. In this study, the wavefunction is a superposition of the ground state and the first two excited states. It is necessary to consider three eigenstates because if we consider only two eigenstates, the Bohmian trajectory produced is only dependent on one frequency for which there is no chaos occur [8]. Besides that, we choose the first three eigenstate because these states are the most stable ones [15]. Taking a linear combination of the eigenstates, we got the time of evolution resulting the wavefunction which is given by

$$\left(\frac{\alpha A e^{-i(\omega_1+\omega_2)t}}{\sqrt{\pi}} + \frac{2x\alpha B e^{-\frac{i}{2}(\omega_1+3\omega_2)t}}{\sqrt{2\pi}} + \frac{2y\alpha C e^{-i(3\omega_1+\omega_2)t}}{\sqrt{2\pi}}\right) e^{\frac{1}{2}(\omega_1 x^2 + \omega_2 y^2)} \tag{13}$$

where $A = \mathrm{a} + id$, $B = \mathrm{b} + ig$, $C = \mathrm{f} + ic$. These complexes numbers must satisfy the normalization condition $|A| + |B| + |C| = 1$. By substituting Eq. (13) into Eq. (11), we obtained the velocity of the particle,

$$v_x = -\frac{\sqrt{2}\alpha^2\beta_x - 2\alpha^2\gamma_x y}{V(x,y,t)} \tag{14}$$

$$v_y = -\frac{\sqrt{2}\alpha^2\beta_y - 2\alpha^2\gamma_y x}{V(x,y,t)} \tag{15}$$

where,

$$\beta_x = (ab + dg)Sin(\omega_2 t) - (ag - bd)Cos(\omega_2 t)$$

$$\beta_y = (af + dg)Sin(\omega_1 t) - (ag - bd)Cos(\omega_1 t)$$

$\gamma_x = (bf + gc)Cos(\omega_1 - \omega_2)t + (bc - gf)Cos(\omega_1 - \omega_2)t$

$\gamma_y = (bf + gc)Cos(\omega_1 - \omega_2)t - (bc - gf)Cos(\omega_1 - \omega_2)t$

$V(x, y, t) = 2x^2\alpha^2(b^2 + g^2) + 2y^2\alpha^2(c^2 + f^2) + \alpha^2(a^2 + d^2)$

$+2\sqrt{2}\alpha^2[(ab + dg)Cos(\omega_2 t) + (ag + bd)Sin(\omega_2 t)]x$

$+2\sqrt{2}\alpha^2[(af + dc)Cos(\omega_1 t) + (ac + df)Sin(\omega_1 t)]y$

$+4\alpha^2[(bf + gc)Cos(\omega_1 - \omega_2)t + (bc + gf)Sin(\omega_1 - \omega_2)t]xy$

and these two differential form were solved from the quantum trajectories which had defined in Bohmian framework.

4. Method

Lyapunov exponent provide the rate of exponential divergence or convergence of infinitesimally close trajectories for a dynamical system. Benettin *et al.,* [16] had proposed a method to do in numerical calculation by computing the Lyapunov exponents for bounded systems. Two nearby points in phase space M are considered with very small separation.

$$|\delta p_0| = \|x_0 - y_0\| \tag{16}$$

where $\|\dots\dots\|$ is the Euclidean norm and x_0 and y_0 are initial point of two nearby trajectories. After that, for any time t $\in\Re$, we can define the Hamiltonian flow $\{T^t\}$ given by

$$x(t) = T^t x_0 \tag{17}$$

$$y(t) = T^t y_0 \tag{18}$$

Hence, the distance between these two trajectories at time t is

$$|\delta p_t| = \|x(t) - y(t)\| \tag{19}$$

We need to modify Eq. (17) and Eq. (18) in order to maintain the trajectories separation within the linearized flow range, for given a fixed time t, these equations become

$$x_i = T^t x_{i-1} \tag{20}$$

$$y_i = T^t y_{i-1} \tag{21}$$

where $i \in \aleph$ and Eq. (19) turn into

$$|\delta p_t| = \|T^t x_{i-1} - T^t y_{i-1}\| \tag{22}$$

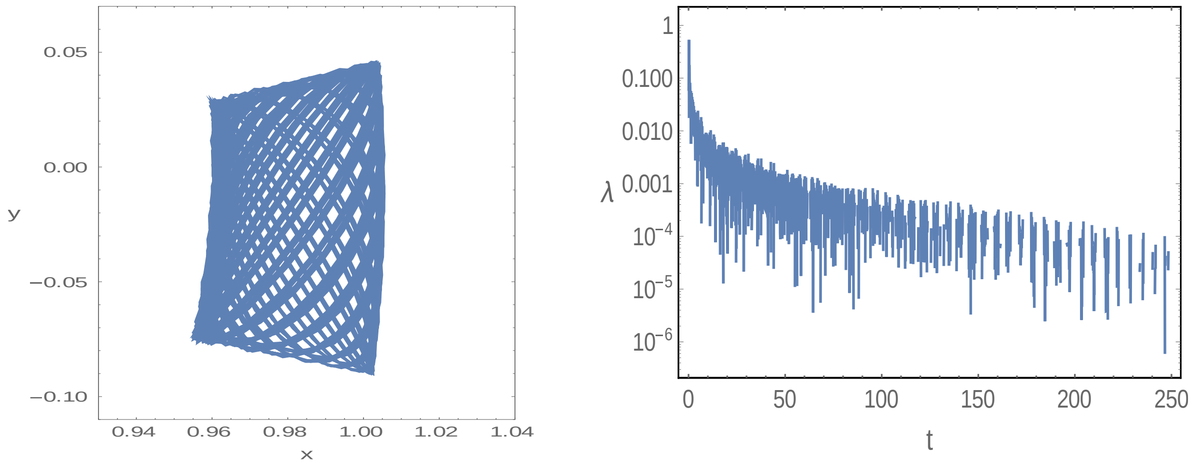
In this way, we can define $x_1 = T^t x_0$ and $|\delta p_1| = \|T^t x_0 - T^t y_0\|$. Afterwards we have to rescale y_i so that $\|y_1 - x_1\| = |\delta p_0|$. This procedure will be repeated by m times to obtain a series of positive number $\{\delta p_i\}$ and the Lyapunov exponent given by

$$\lambda = \frac{1}{t}\sum_{i=1}^{m} ln\frac{|\delta p_i|}{|\delta p_0|} \quad (23)$$

5. Results

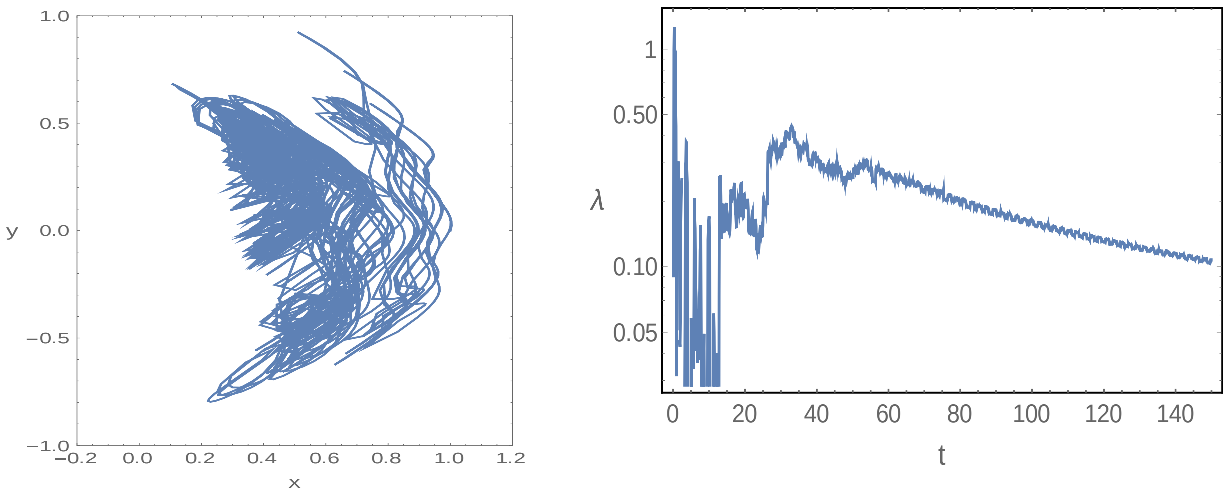
We successfully run the developed programs for four different sets of initial conditions and combination of 30 different values of frequency. Therefore, the focus of this paper is to quantitatively and qualitatively describe the results in term of the relation between frequency ratios, mixture of amplitude and the behaviour of the system.

According to our results, most of the relationship between frequency ratios and behaviour of the system is hard to explain quantitatively. For example, if we increase or decrease the frequency ratios, the behaviour of the system does not gradually change from regular to chaos or from chaos to regular. It is unfortunate that, we cannot directly describe mathematically the connection between them because functions x[t] and y[t] are not known explicitly since Eq. (14) and Eq. (15) are unsolvable analytically. However, we found that, at certain conditions of frequency ratios, there exists a clear qualitative relation between frequency ratios and the onset of chaos. Let us consider $\omega_2 > \omega_1$ and $\omega_2 \geq 10$ Hz. In Figure 1(a), we show that when the frequency ω_1 is much smaller than ω_2, the Bohmian trajectory is regular (Figure 1(b)). However, when we increase the value of ω_1 approaching the value of ω_2, the Bohmian trajectory gradually changes to disordered pattern and exhibits chaos (Figures 2(a) and 2(b)).



(a) (b)

Fig. 1. (a) A Bohmian orbit with initial condition x_0= 1, y_0 = 0, a = 0.37, b = 0.44, c = 0.44, d = -0.02, e = 0.49, f = -0.49 for frequencies ratio 1:20. (b) The time evolution of the Lyapunov exponent

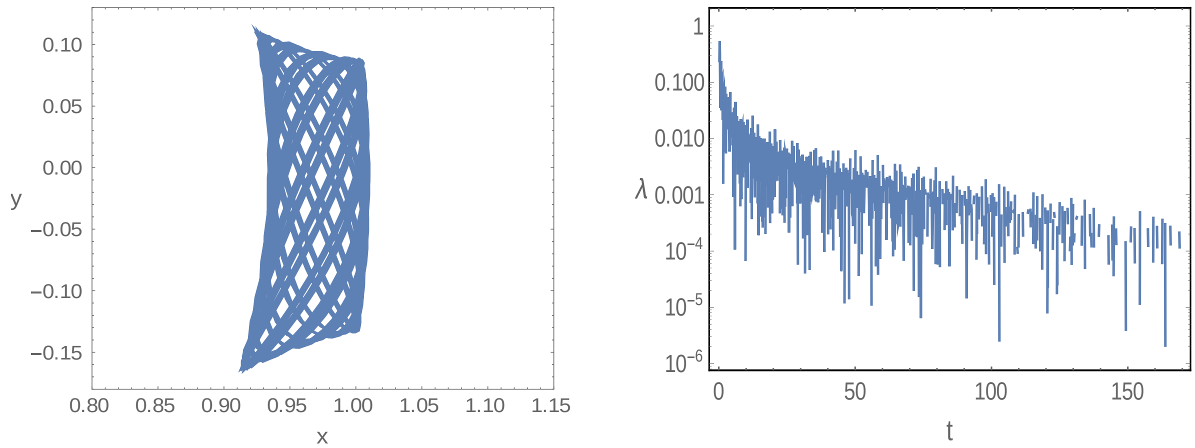


(a) (b)

Fig. 2. (a) A Bohmian orbit with initial condition x_0= 1, y_0 = 0, a = 0.37, b = 0.44, c = 0.44, d = -0.02, e = 0.49, f = -0.49 for frequencies ratio 17:20. (b) The time evolution of the Lyapunov exponent

This onset also occurs when ω_1 is greater than ω_2. Therefore, in this case, we can say that, the system exhibits chaos when frequency ratios approach to 1 and when at least one of the frequencies have greater value than 10 Hz. This means that, to generate chaos, high frequencies are needed and more or less both frequencies have equal values. As discussed above, the behaviour of the system is strongly dependent on frequency ratios, we found that the relationship is only valid in a finite range of frequency ratios.

We found that if ω_2 is much greater than ω_1 or vice versa, the trajectory forms an ordered pattern (Figure 3(a)) and hence exhibits regular motion (Figure 3(b)). According to our results, the system may exhibit chaos when 1Hz $\geq |\omega_2 - \omega_1| \geq$ 5Hz. In order to understand this, let us express the first three eigenstates in term of frequency ratios.



(a) (b)

Fig. 3. (a) A Bohmian orbit with initial condition x_0= 1, y_0 = 0, a = 0.37, b = 0.44, c = 0.44, d = -0.02, e = 0.49, f = -0.49 for frequencies ratio 3:13. (b) The time evolution of the Lyapunov exponent

$$
\begin{aligned}
\psi_{0,0} &= \frac{\alpha}{\sqrt{\pi}} e^{\frac{1}{2}(\omega_1 x^2 + \omega_2 y^2)} e^{-\frac{i\omega_2}{2}\left(1+\frac{\omega_1}{\omega_2}\right)t} \\
\psi_{0,1} &= \frac{2y\alpha}{\sqrt{\pi}} e^{\frac{1}{2}(\omega_1 x^2 + \omega_2 y^2)} e^{-\frac{i\omega_2}{2}\left(3+\frac{\omega_1}{\omega_2}\right)t} \\
\psi_{1,0} &= \frac{2x\alpha}{\sqrt{\pi}} e^{\frac{1}{2}(\omega_1 x^2 + \omega_2 y^2)} e^{-\frac{i\omega_2}{2}\left(\frac{1}{3}+\frac{\omega_1}{\omega_2}\right)t}
\end{aligned} \tag{24}
$$

When ω_2 is much greater than ω_1, the term ω_1/ω_2 will approach zero. Therefore, in this situation, we assume that the system is not dependent on the frequency ratio but only on the dominant frequency ω_2. As mentioned earlier, the system cannot generate chaos if it only depends on a single value of frequency.

This result may become a motivation for the other study to examine the distinction between the behaviour of classical system and its quantum counterpart. For example, we can make a comparison between the chaotic system governed by Navier-Stokes equations simulated by the immersed boundary method [17] with the corresponding quantum system using the Bohmian mechanics. Besides that, it may be contributed to the clear description about the physical phenomena such as the heat transfer in nanofluids. Due to the very small size of nanoparticles, the quantum effects [18] and the chaotic movements [19] of nanoparticles might be an important mechanism in explaining the nanofluid heat transfer augmentation. One of the possible studies is to extend the work done by Tan *et al.,* [20] which may explain the diffusivity of nanoparticle to enhance the thermal properties in terms of chaos in Bohmian framework.

6. Conclusions

Although Bohmian mechanics is based on trajectories, several factors like frequency ratios, number of eigenstates of wavefunction and degree of freedom make the system in Bohmian framework behave differently in comparison to classical mechanics which is well known integrable system. For the case of frequency ratios, most of the relation between frequency ratios and behaviour of the system is hard to explain quantitatively. For example, if we increase or decrease the frequency ratios, the behaviour of the system does not gradually change from regular to chaos or from chaos to regular. Unfortunately, because of functions x[t] and y[t] are not known explicitly since Eq. (14) and Eq. (15) are unsolvable analytically, we cannot directly describe mathematically the connection between them. In other words, both of them are not proportional to each other. However, in certain conditions which are $\omega_2 > \omega_1$, 1Hz $\geq |\omega_2 - \omega_1| \geq$ 5Hz and $\omega_2 \geq$ 10 Hz, we found a clear relation between frequency ratios and the behaviour of the system. The system changes from regular to chaotic behaviour when ω_1 approaches ω_2.

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