Action principle for cellular automata and the linearity of quantum mechanics

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(Received 3 September 2013; published 15 January 2014)

We introduce an action principle for a class of integer-valued cellular automata and obtain Hamiltonian equations of motion. Employing sampling theory, these discrete deterministic equations are invertibly mapped on continuum equations for a set of bandwidth-limited harmonic oscillators, which encode the Schrödinger equation. Thus, the linearity of quantum mechanics is related to the action principle of such cellular automata and its conservation laws to discrete ones.

DOI: 10.1103/PhysRevA.89.012111 PACS number(s): 03.65.Ca, 03.65.Ta, 03.67.−a, 45.05.+x

I. INTRODUCTION

The linearity of quantum mechanics (QM) is obvious in the Schrödinger equation and similarly in its functional form in quantum field theory (QFT). It is a fundamental aspect that does not depend on the object under study, if it is sufficiently isolated from anything else. Most importantly, by way of the superposition principle, linearity entails such "quantum essentials" as interference and entanglement. They are at the core of QM and of its applications alike, e.g. in advanced precision measurement and information technologies.

Nevertheless, linearity of QM has been questioned from time to time, and particular nonlinear modifications have been proposed. They have been subjected to experimental tests, putting bounds on their parameters when none of their predicted effects have been seen. Ample discussion and a stepwise proof that QM has to be linear have been provided by Jordan, based on the separability assumption "that the dynamics we are considering can be independent of something else in the universe, that the system we are considering can be described as part of a larger system without interaction with the rest of the larger system" [1]. In Weinberg's articles, for example, a class of modifications and their relation to experimental signatures have been studied [2]. In this case, theoretical objections have been raised, showing that the proposed nonlinearities would lead to superluminal signals or communication between branches of the wave function [3,4]; since then, "no signaling" has become a versatile criterium confronting attempted modifications of QM [5].

The purpose of this article is to demonstrate a relation between QM and mechanics of a class of Hamiltonian cellular automata. In this way, the linearity of QM becomes an unavoidable feature deriving from the action principle governing the discrete dynamics.

This is motivated by explorations of discrete deterministic mechanics by Lee [6], by the study of bandwidth-limited fields and their possible role in discrete structures on and of spacetime by Kempf [7], and by the representation of QM in terms of classical notions of observables, phase space, and Poisson bracket algebra by Heslot [8,9]. A combination of these ideas promises to be fruitful for our understanding of interference, entanglement, and measurement in QM and for new approximation schemes in quantum theory.

II. DISCRETE HAMILTONIAN MECHANICS

Discreteness arises in many contexts in physics or mathematics, besides quantization, e.g., in discrete maps facilitating numerical studies of complex systems, as regularized versions of quantum field theories on spacetime lattices, or describing intrinsically discrete processes. Finite difference equations can be expected to play a role here, diminishing the preponderance of differential calculus.

Lee and collaborators proposed to incorporate fundamental discreteness into all of dynamics [6] (and references therein), witnessing the difficulties in trying to find a manageable theory of "quantum gravity," let alone "the" unified theory. Deterministic discrete mechanics derives from the assumption that *time is a discrete dynamical variable*. This invokes a *fundamental length or time scale* (in natural units), l, and can be more aptly phrased that in a fixed $(d+1)$-dimensional spacetime volume Ω maximally Ω/l^{d+1} measurements can be performed or this number of events take place.

Various models have been elaborated which share desirable symmetries with the corresponding continuum theories while presenting finite degrees of freedom. Different forms and (dis)advantages of a Lagrangian formulation [6] have been discussed, e.g., in Refs. [10–12]. Instead, we introduce an action principle which leads to particularly transparent and symmetric Hamiltonian equations of motion. This induces a discrete phase space picture of the dynamics.

Consider a classical cellular automaton (CA) with a denumerable set of degrees of freedom and represent its state by *integer-valued* "coordinates" x_n^α,τ_n and "conjugated momenta" p_n^α,π_n, where $\alpha\in\mathbf{N}_0$ denote different degrees of freedom and $n\in\mathbf{Z}$ different states. (The x_n and p_n might be higher dimensional vectors, while τ_n and $\mathcal{P}_n$ are assumed one-dimensional.) Finite differences, for all dynamical variables, are defined by

$$\Delta f_n := f_n - f_{n-1}. \tag{1}$$

Furthermore, we define (using henceforth the summation convention for Greek indices, $r^\alpha s^\alpha \equiv \sum_\alpha r^\alpha s^\alpha$)

$$\mathcal{A}_n := \Delta\tau_n(H_n + H_{n-1}) + a_n, \tag{2}$$

$$H_n := \frac{1}{2}S_{\alpha\beta}\left(p_n^\alpha p_n^\beta + x_n^\alpha x_n^\beta\right) + A_{\alpha\beta}p_n^\alpha x_n^\beta + R_n, \tag{3}$$

$$a_n := c_n\pi_n, \tag{4}$$

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where constants, c_n, and symmetric, $\hat{S} \equiv \{S_{\alpha\beta}\}$, and antisymmetric, $\hat{A} \equiv \{A_{\alpha\beta}\}$, matrices are all integer-valued; R_n stands for higher than second powers in x_n^α or p_n^α. The choice of a_n influences the behavior of the variable τ_n; we consider here only a very simple possibility [13].

Defining the integer-valued CA *action*:

$$\mathcal{S} := \sum_n \left[\left(p_n^\alpha + p_{n-1}^\alpha\right)\Delta x_n^\alpha + (\pi_n + \pi_{n-1})\Delta\tau_n - \mathcal{A}_n \right], \quad (5)$$

the evolution of the CA is determined by this:

Postulate. The CA follows the discrete updating rules (equations of motion) which are determined by the *action principle* $\delta\mathcal{S} = 0$, referring to arbitrary integer-valued variations of all dynamical variables defined by

$$\delta g(f_n) := [g(f_n + \delta f_n) - g(f_n - \delta f_n)]/2, \quad (6)$$

where f_n stands for one of the variables on which polynomial g may depend. ■

Several remarks are in order here. First, we observe that the variations of constant, linear, or quadratic terms yield results that are analogous to the continuum case. Second, while infinitesimal variations do not conform with integer valuedness, there is no *a priori* constraint on integer ones. However, for arbitrary δf_n, the *remainder of higher powers* in Eq. (3), which enters the action, has to vanish for consistency, $R_n \equiv 0$. Otherwise the number of equations of motion generated by the action principle, generally, would exceed the number of variables [14].

Introducing the notation $\dot{O}_n := O_{n+1} - O_{n-1}$, the following CA *equations of motion* are obtained:

$$\dot{x}_n^\alpha = \dot{\tau}_n\left(S_{\alpha\beta}p_n^\beta + A_{\alpha\beta}x_n^\beta\right), \quad (7)$$

$$\dot{p}_n^\alpha = -\dot{\tau}_n\left(S_{\alpha\beta}x_n^\beta - A_{\alpha\beta}p_n^\beta\right), \quad (8)$$

$$\dot{\tau}_n = c_n, \quad (9)$$

$$\dot{\pi}_n = \dot{H}_n, \quad (10)$$

which are discrete analogues of Hamilton's equations, where all terms are defined in terms of integers. The discrete *automaton time* n is reflected by the finite difference equations here.

Note that $\dot{\tau}_n$ present *background* parameters for the evolving x, p variables, as a consequence of Eqs. (4) and (9). Generally, $\dot{\tau}$ is a *lapse function* in Eqs. (7)–(8).

Equations (7)–(10) are *time reversal invariant*; the state $n+1$ can be calculated from knowledge of the earlier states n and $n-1$ and the state $n-1$ from the later ones $n+1$ and n.

Furthermore, there are conservation laws that are always respected by Eqs. (7)–(8).–Introducing the self-adjoint matrix $\hat{H} := \hat{S} + i\hat{A}_{\alpha\beta}$, these equations yield

$$\dot{x}_n^\alpha + i\dot{p}_n^\alpha = -i\dot{\tau}_n H_{\alpha\beta}\left(x_n^\beta + ip_n^\beta\right) \quad (11)$$

and its adjoint. Thus, we recover a *discrete analog of Schrödinger's equation*, with $\psi_n^\alpha := x_n^\alpha + ip_n^\alpha$ as the amplitude of the "α component" of "state vector" $|\psi\rangle$ at "time" n. Then, Eqs. (7)–(8) imply this:

Theorem A. For any matrix $\hat{G}$ that commutes with $\hat{H}$, $[\hat{G},\hat{H}] = 0$, there is a *discrete conservation law*:

$$\psi_n^{*\alpha}G_{\alpha\beta}\dot{\psi}_n^\beta + \dot{\psi}_n^{*\alpha}G_{\alpha\beta}\psi_n^\beta = 0. \quad (12)$$

For self-adjoint $\hat{G}$, with complex integer elements, this relation concerns real integer quantities. ■

Corollary A. For $\hat{G} := \hat{1}$, Eq. (12) implies a *conserved constraint* on the state variables:

$$\psi_n^{*\alpha}\dot{\psi}_n^\alpha + \dot{\psi}_n^{*\alpha}\psi_n^\alpha = 0. \quad (13)$$

For $\hat{G} := \hat{H}$, an *energy conservation* law follows. ■

Such matrices $\hat{G}$ generate *discrete unitary symmetry transformations*; admissible ones preserve complex integer valuedness of the CA variables ψ_n^α.

Note that Eqs. (12) and (13) *cannot* be trivially "integrated," since the *Leibniz rule* is modified. Recalling $\dot{O}_n := O_{n+1} - O_{n-1}$, we have, for example, $O_{n+1}O'_{n+1} - O_{n-1}O'_{n-1} = \frac{1}{2}(\dot{O}_n[O'_{n+1} + O'_{n-1}] + [O_{n+1} + O_{n-1}]\dot{O}'_n)$, instead of the product rule of differentiation.

Furthermore, we cannot obtain a continuum limit simply by letting the discreteness scale $l \to 0$, as, for example, in Refs. [6,15]. Integer valuedness here conflicts with continuous time and related derivatives.

It is worth recalling the underlying assumption of discrete mechanics that the density of events and, thus, of information content of spacetime regions is cut off by the scale l [6,16]. We may wonder whether the discreteness of a deterministic CA can be reconciled with any continuum description at all and, in particular, with QM.

III. SAMPLING THEORY

We propose an answer here by exploring the possibility that physical fields, wave functions in particular, could be *simultaneously discrete and continuous*, represented by sufficiently smooth functions containing a finite density of degrees of freedom. This idea has recently been introduced by Kempf and has led to constructing a covariant ultraviolet cutoff suitable for theories including gravity, with motivation provided by ubiquitous appearance of generalized uncertainty relations [7]. However, neither *integer-valued CA* nor the *structure of QM* have been addressed in this context.

In his pioneering work, Shannon pointed out that information can have simultaneously continuous and discrete character [17]. This has become a matter of routine application in signal processing, whenever conversion between analog and digital encoding is needed. Sampling theory demonstrates that any bandlimited signal can be perfectly reconstructed, provided discrete samples of it are taken at the rate of at least twice the band limit (Nyquist rate). For an extensive review, see Ref. [18]; see also Ref. [19], referring to modern ramifications of the theory.

For our present purposes, the *Sampling Theorem* in its simplest form suffices [7,18]: Consider square integrable *bandlimited functions* f, i.e., which can be represented as $f(t) = (2\pi)^{-1}\int_{-\omega_{\max}}^{\omega_{\max}} d\omega\, \mathrm{e}^{-i\omega t}\tilde{f}(\omega)$, with bandwidth $\omega_{\max}$. Given the set of amplitudes $\{f(t_n)\}$ for the set $\{t_n\}$ of equidistantly spaced times (spacing $\pi/\omega_{\max}$), the function f is obtained for all t by

$$f(t) = \sum_n f(t_n)\frac{\sin[\omega_{\max}(t-t_n)]}{\omega_{\max}(t-t_n)}. \quad (14)$$

Since the CA time is given by the integer n, the corresponding discrete *physical time* is obtained by multiplying with the fundamental scale l, $t_n \equiv nl$, and the bandwidth by $\omega_{\max} = \pi/l$.

Attempting to *map invertibly* Eqs. (7)–(8) on reconstructed continuum equations, according to Eq. (14), the nonlinearity on the right-hand sides is problematic: the product of two functions, with bandwidth $\omega_{\max}$ each, is not a function with the same bandwidth. Therefore, the mapping can only be consistent if $\dot{\tau}_n$ is a constant.

Let us recall Eq. (11). Inserting $\psi_n^\alpha := x_n^\alpha + ip_n^\alpha$ and applying the *Sampling Theorem*, this discrete time equation is mapped to the *continuous time equation*:

$$\frac{\hat{D}_l - \hat{D}_{-l}}{2}\psi^\alpha(t) = \sinh(l\partial_t)\psi^\alpha(t) = \frac{1}{i}H_{\alpha\beta}\psi^\beta(t), \quad (15)$$

where we employed the translation operator defined by $\hat{D}_T f(t) := f(t+T)$ and set $\dot{\tau}_n \equiv \dot{\tau} = 2$ [20].

Thus, we obtain the *Schrödinger equation*, however, modified in important ways. (We use QM terminology freely, while paying attention to new effects arising here.) The wave function ψ^α has bandwidth $\omega_{\max}$, due to reconstruction formula (14). This corresponds to an *ultraviolet cutoff* of the energy E of stationary states of the generic form $\psi_E(t) := \exp(-iEt)\tilde{\psi}$. Indeed, diagonalizing the self-adjoint Hamiltonian, $\hat{H} \to \mathrm{diag}(\epsilon_0,\epsilon_1,\ldots)$, Eq. (15) yields the eigenvalue equation:

$$\sin(E_\alpha l) = \epsilon_\alpha \quad (16)$$

and a *modified dispersion relation*, $E_\alpha = l^{-1}\arcsin(\epsilon_\alpha) = l^{-1}\epsilon_\alpha[1 + \epsilon_\alpha^2/3! + O(\epsilon_\alpha^4)]$ [21]. The spectrum $\{E_\alpha\}$ is cut off by the condition $|\epsilon_\alpha| \leqslant 1$, entailing $|E_\alpha| \leqslant \pi/l = \omega_{\max}$, i.e., the bandlimit.

The modified Schrödinger equation (15) incorporates higher-order time derivatives. These are negligible for low-energy wave functions, which vary little with respect to the cutoff scale, i.e., $|\partial^k\psi/\partial t^k| \ll l^{-k} = (\omega_{\max}/\pi)^k$.

Furthermore, the relation between Eq. (11) and Eq. (15), together with the linearity of both equations, suggest that the correct continuous time conservation laws are obtained by the replacement:

$$\dot{\psi}_n := \psi_{n+1} - \psi_{n-1} \quad \longrightarrow \quad \frac{1}{i}\sin(il\partial_t)\psi(t); \quad (17)$$

cf. Eqs. (12) and (13), respectively. Indeed, by Eq. (15), the following holds:

Theorem B. For any matrix $\hat{G}$ that commutes with $\hat{H}$, there is a *continuous time conservation law*:

$$\psi^{*\alpha}G_{\alpha\beta}\sin(il\partial_t)\psi^\beta + [\sin(il\partial_t)\psi^{*\alpha}]G_{\alpha\beta}\psi^\beta = 0, \quad (18)$$

in particular,

$$\psi^{*\alpha}\sin(il\partial_t)\psi^\alpha + [\sin(il\partial_t)\psi^{*\alpha}]\psi^\alpha = 0, \quad (19)$$

which appropriately modifies the QM wave function *normalization*, referring to a basis denumerated by α. ■

Equations (18)–(19) allow us to remove the ultraviolet cutoff, $l \to 0$, recovering QM results from the leading order terms. (If l is a fundamental *constant*, this limit may be interesting for heuristic reasons alone.) For example, consider the real symmetric *two-time function*,

$$2C_{\hat{G}}(t_1,t_2) := \psi^{*\alpha}(t_1)G_{\alpha\beta}\psi^\beta(t_2) \; + \; \text{c.c.}, \quad (20)$$

where $X + \text{c.c.} := X + X^*$ and $\hat{G}$ is a self-adjoint matrix, with $[\hat{G},\hat{H}] = 0$. Inserting $C_{\hat{G}}$, Theorem B yields:

Corollary B. The two-time function $C_{\hat{G}}$ is invariant under discrete translations of this form:

$$C_{\hat{G}}(t-l,t) = C_{\hat{G}}(t,t+l), \quad (21)$$

implying that it is fixed everywhere by giving $C_{\hat{G}}(t,t+l)$ for all t in an interval $[t_0,t_0+l[$. ■

The wave function normalization, $\psi^{*\alpha}\psi^\alpha = 1$, then arises here from the coincidence limit of a two-time function with the property $C_{\hat{1}}(t,t+l) \equiv 1$, for all t:

$$1 = \lim_{l\to 0} C_{\hat{1}}(t,t+l) = \psi^{*\alpha}(t)\psi^\alpha(t), \quad (22)$$

which is consistent with Eq. (19) and essential for the probability interpretation in QM. An analogous *equal-time* constraint, in general, does not exist on the CA level of description. For example, $\psi_n^{*\alpha}\psi_n^\alpha = x_n^\alpha x_n^\alpha + p_n^\alpha p_n^\alpha = 1$, instead of Eq. (13), is compatible only with rather trivial evolution, since all variables are integer-valued.

It is remarkable how properties of CA produce familiar QM results, even if modified by the finite scale l. Matrices that generate QM conservation laws do so for the bandwidth-limited continuum theory. Since the *same* vanishing commutator is responsible for CA conservation laws, Eqs. (12)–(13), they strictly correspond to each other. Yet continuous QM symmetry transformations, generally, comprise a larger set than discrete CA ones respecting complex integer valuedness.

IV. DISCUSSION

It will be interesting to find a similar one-to-one CA–QM map for relativistic QM and QFT. Since wave equations and functional Schrödinger equation are linear and have a Hamiltonian formulation, it should be possible to employ a generalized *Sampling Theorem* for fields. It has been shown how to covariantly regularize the d'Alembert operator by finite bandwidth of its spectrum [7], which is a necessary ingredient. Conversely, given a *Hamiltonian* CA, we may invoke the path integral for classical systems [22], with integration replaced by summation over integer-valued variables, plus reconstruction formulas, in order to derive a relativistic bandwidth-limited quantum (field) theory. Other constructions of CA for *relativistic models* have appeared which either incorporate QM features from the outset, e.g., for the Dirac equation [23], or derive them, e.g., for bosonic QFT and a superstring model [24]; see also references in those papers. These models have been all *noninteracting*.

Lack of interactions there seems dictated by additional restrictions, such as locality, due to placing a CA, say, at Planck scale, into physical spacetime as experienced at scales where QM is tested. Remarkably, arbitrary QM N-level systems can be described by $2N-1$ nonrelativistic coupled oscillators in one fictitious space dimension [25]. Are these hints that fundamental CA exist in an abstract space and that QM and spacetime emerge from there?

The nonrelativistic CA considered in this article *do* incorporate *interactions* through matrix elements $H_{\alpha\beta}$. Their x^α, p^α variables can be embedded into two-dimensional phase space, similarly as in Ref. [25]. Yet other interpretations are possible, such as α labeling sites of a d-dimensional lattice or, generally, elements of a Hilbert space in the QM description following *sampling theory*. This freedom is due to the nonrelativistic formalism without reference to gravitation or dynamical spacetime.

The only other known approach allowing for interactions is a statistical theory of certain matrix models, which shows QM behavior to emerge from a Gibbs distribution [26]. Similarly as in Refs. [24], however, this assumes a particular dynamics, and it remains to be seen whether gauge theories as, for example, in the Standard Model can be covered. Our approach here, in distinction, does not make assumptions about specific interactions or forces but explores a mapping between structural features of Hamiltonian CA and of QM. It will be challenging to identify the principles that govern a physically relevant Hamiltonian $\hat{H}$ within the "ontology" of CA.

It is worth while to also draw attention to the essential feature of *entanglement* in QM, as well as to the often discussed apparent nonlocality, and how this is reflected on the CA level.

Considering the apparent nonlocality, we may refer here to recent work demonstrating that QM is a local theory in a well-defined sense, while much of ongoing debates must be attributed to terms which are imprecisely defined or used with varying connotations [27]. Concerning this, however, our mapping between CA and QM does *not* change QM, except by introducing the fundamental parameter l in correction terms to Schrödinger equation and corresponding conservation laws. These modifications are negligible in the realm where QM has been tested, if l belongs to the Planck scale. Therefore, arguments brought forth in the discussion of locality in QM, especially in Ref. [27], apply here to the same extent.

Entanglement is present in our theory as in QM, since it arises as a consequence of its *linearity* embodied in the *superposition principle*, which has been main topic of this article. More specifically, there can be entangled states, when the relevant Hilbert space is a tensor product of subspaces. Which, in the simplest case, allows to have superposition "Bell" states, e.g., $|\psi\rangle = |\alpha\rangle \otimes |\beta\rangle \pm |\beta\rangle \otimes |\alpha\rangle$, where the first factor of the tensor products belongs to a subspace "A" and the second to a subspace "B." This type of structure, or its generalizations, can be built in our linear theory as well, and even on the CA level where the theory is again linear. We have not explicitly discussed tensorized spaces, when introducing wave function components ψ^α referring to a Hilbert space with denumerable basis, nor when introducing canonically conjugated x^α, p^α variables for CA. Which is motivated by the fact that the tensorized structure can always be embedded in a sufficiently large Hilbert space, such that it is *de facto* absent, but is reflected in a corresponding change of the algebra of observables. This has been elaborated in detail recently, because of the relevance for quantum information protocols. A concise exposition for the case of overall pure states is in Ref. [28]. We conclude that our theory does not produce deviations from QM that would affect entanglement, which remains a manifestation of the linearity on both levels, CA as well as QM.

It will be most interesting to reconsider questions of entanglement and locality, when a relativistic generalization of the present theory becomes available.

Observables, measurements, and Born rule can be discussed in bandwidth-limited theory with help of Heslot's work [8] and implications for CA be considered elsewhere.

Our results suggest to simulate complex QM systems by mapping on computer-friendly integer-valued Hamiltonian CA. The CA updates are *error free*. Introducing a bandwidth, rescaling the modified Schrödinger equation followed by mapping Hamiltonian matrix elements approximately on complex integer ones, and finite time effects produce errors to be explored; *cf.* the last of Ref. [23].

We remark that Planck's constant $\hbar$ does not interfere with such a map and remains independent here of the discreteness scale l. This can be illustrated as follows. We write the Schrödinger equation in the form $i\hbar\partial_{t'}\psi = \epsilon_{\mathrm{phys}}\hat{h}\psi$, where by ϵ_{phys} we factor out the physical energy scale of the problem at hand, such that the dimensionless Hamiltonian $\hat{h}$ is given by numbers that are (loosely speaking) "of $O(1)$." Rescaling the time variable $t'/M' =: t$, with $M' \gg 1$, we obtain $i\hbar\partial_t\psi = \epsilon_{\mathrm{phys}}M'\hat{h}\psi = (\hbar\omega_{\mathrm{max}}/\pi)M\hat{h}\psi$, where we introduced the bandwidth limit, $\hbar\omega_{\mathrm{max}}/\pi := \epsilon_{\mathrm{phys}}M'/M$, with $M' \gg M \gg 1$. At this point, units can be chosen such that $\hbar = 1$, as usual. Furthermore, we introduce a complex integer-valued Hamiltonian, $\hat{H} := M\hat{h}$, as an approximation on the right-hand side of the Schrödinger equation, which may introduce errors for its matrix elements (loosely speaking) "of $O(1/M)$." This presents the starting point for an analysis invoking sampling theory, in order to map the dynamics on a cellular automaton.

V. CONCLUSION

In conclusion, a map between cellular automata (CA) and quantum mechanics (QM) has been constructed by a synthesis of elements from *discrete mechanics* [6], *sampling theory* [7], and *Hamiltonian formulation* of QM [8]. QM can originate in integer-valued CA incorporating a fundamental scale. The postulated action principle refers to (the only available) arbitrary integer variations of dynamical variables, which enforces the *linearity* of the theory. The *separability assumption* mentioned in Sec. I, which underlies an intrinsic derivation of the linearity of QM [1], can be substituted by another statement in the present context: "the dynamics we are considering can be independent of something else in the universe," if and only if the relevant CA *action is stationary under arbitrary integer variations*. This may open another view of linearity and the superposition principle in quantum mechanics.

ACKNOWLEDGMENTS

It is a pleasure to thank N. Buric and T. E. Skinner for critical reading and suggestions concerning a preliminary version of this paper, A. Kempf for feedback, and an anonymous referee for careful remarks.

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