Microscopic foundations of the Second Law of Thermodynamics within Nonunitary Newtonian Gravity

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Abstract

The quest for a microscopic foundation of thermodynamics is addressed within the Nonunitary Newtonian Gravity model through the study of a specific closed system, namely a three-dimensional harmonic nanocrystal. A numerical calculation of the nanocrystal von Neumann entropy as a function of time is performed, showing a sharp monotonic increase, followed by a stabilization at late times. This behavior is consistent with the emergence of a micro-canonical ensemble within the initial energy levels, signaling, in this way, the establishment of a nonunitary gravity-induced thermal equilibrium.

keywords: Gravity; entanglement entropy; thermalization.

1 Introduction

The two weak points of the final setting of Quantum Mechanics (QM) by von Neumann, the vague notion of a macroscopic measurement apparatus and the definition of coarse graining entropy, based, as it is, on the subjective notion of macroscopic observables, can in principle both be addressed by a nonunitary quantum dynamics. The natural way to get a nonunitary dynamics is to put the physical system in interaction with an ancillary system and then tracing out the ancilla to get a mixed state described by a density matrix, just as it happens with open systems when environment is traced out. If we want to identify thermodynamic entropy with the entanglement entropy with an ancillary or hidden system [1, 2, 3], we have at least to require thermal equilibrium between the physical system and the hidden one:

\[ \frac{1}{T} = \frac{\partial S}{\partial E_p} - \frac{\partial S}{\partial E_h} = \frac{\partial S}{\partial E_p} \left( \frac{\partial E_h}{\partial E_p} \right)^{-1}, \]  

(1)

where \( E_p \) and \( E_h \) denote respectively the energy of the physical and the hidden system, while the entropy \( S \) is one and the same for the two systems, being the entanglement entropy of a bipartite system.

The above thermal equilibrium condition leads to the almost inescapable conclusion that every physical system must have as hidden partner its exact replica and the metasystem (physical plus hidden) state space must be restricted by a symmetry constraint in the exchange of physical and hidden degrees of freedom. This constraint eliminates the arbitrariness of considering as non observable some degrees of freedom, since in any constrained theory, like Gupta-Bleuler’s, the observable algebra is a subalgebra of the original dynamical one.

Several models were proposed to modify quantum dynamics in order to get localization and transition to classicality, and some of them tried to establish a link with gravity [4, 5, 6, 7]. They all introduced phenomenological parameters, while for a fundamental theory \( G, h \) and \( c \) should be enough since these three fundamental constants allow one to make all physical entities dimensionless. If we limit ourselves to low energy physics, only \( G \) and \( h \) should appear in an approximate low energy model and, for dimensional reasons, the only possible relation between threshold mass \( M \) and length \( L \) for localization and transition to classicality is

\[ M^3L = \frac{h^2}{G}, \]  

(2)

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which implies that

\[ M = \left( \frac{\hbar^2}{G} \right) \rho \text{vol}. \]

(3)

Here one sees that the dependence on mass density \( \rho \) is exceedingly weak: to get a doubling of \( M \), \( \rho \) has to get \( 2^{10} = 1024 \) times higher. This quasi independence of the threshold mass on mass density could be an experimental signature of gravitational localization.

In Refs. 8, 9, 10, 11 a dynamics was defined and analyzed which gives rise to the same relation as above between threshold mass for localization and mass density. It introduces a gravitational interaction only between a generic physical system and its replica and constraints the metastate space by a symmetry requirement as well. In this model no gravitational interaction was introduced within physical and hidden system as the author had in his mind the possibility to avoid gravitational-collapse singularities. But in Refs. 12, 13 it was shown that a general covariant model, with a sound newtonian limit - differing from the previous one8, 9, 10, 11 just for the inclusion of gravity within the physical and the hidden systems, at ordinary laboratory lengths, and giving about the same localization thresholds - can eliminate gravitational interaction within physical and hidden systems only for lengths of the order of Planck length, thus avoiding collapse singularities.

The low-energy limit of this model, a brief account of which is given in the Appendix A, is known as Nonunitary Newtonian Gravity (NNG, from now on), and has been studied in detail showing (entropic) dynamical self-localization for masses above the sharp threshold of \( 10^{11} \) proton masses, with precise signatures susceptible to future experimental tests 13, 14, 15, 16. Recently it has been explicitly shown to be free from causality violation problems 17, 18, at variance with semiclassical gravity, namely (in the Newtonian limit) Newton-Schroedinger model. Physically this is achieved by decohering linear superpositions of macroscopically distinct states, as a consequence of the dynamical mechanism of state reduction naturally embedded in the model. Another peculiar feature is the evolution of pure states into mixed states even for closed systems 13, 19, so that within NNG density matrix emerges as the fundamental description of physical reality. Indeed, to the best of our knowledge, NNG is the first model treating the density matrix as the fundamental characterization of a closed system state with a non-Markov evolution even from a pure state. In fact on one hand collapse models do not use density matrices as fundamental entities but just as associated to a stochastic evolution, and on the other hand models based on the Lindblad equation give Markov evolution of a mixed state.

All the above features make the NNG model useful to shed new light on the long standing and still open problem of the foundations of the Second Law of thermodynamics 20, 21, 22. Indeed, as pointed out in Ref. 23, starting from suitable initial conditions, only a nonunitary quantum dynamics could allow for a microscopic derivation of the Second Law of thermodynamics for a closed system by resorting to von Neumann entropy.

A first step in demonstrating the ability of NNG to reproduce a gravity-induced relaxation towards thermodynamic equilibrium even for a closed system has been carried out in Ref. 19, by taking a simple system: two particles in an harmonic trap interacting via an ‘electrical’ delta-like potential and gravitational interaction. Starting from an energy eigenstate, a slow net variation of the von Neumann entropy for the system as a whole has to

\[ \text{resulting in a } \Delta E \text{ around } E, \]

according to the prescriptions of the Eigenstate Thermalization Hypothesis (ETH) 24, 25. In this way the behaviour of the von Neumann entropy as a function of time is obtained, which is consistent with the one for a thermalizing system.

The aim of the present paper is to generalize this work to a more complex system, i.e. an harmonic nanocrystal within a cubic geometry. This choice allows us to perform a first step towards the simulation of macroscopic systems where the Second Law of thermodynamics is more relevant. A numerical simulation is carried out by starting from an initial pure physical state with mean energy \( E \), drawn uniformly at random by superposing a huge number of energy eigenstates within the energy interval \( \Delta E \) around \( E \), according to the prescriptions of the Eigenstate Thermalization Hypothesis (ETH) 24, 25. In this way the behaviour of the von Neumann entropy as a function of time is obtained, which is consistent with the one for a thermalizing system.

The plan of the paper is as follows. In Section II we briefly summarize our recent results on the simple two-particle system. In Section III, which is the core of the paper, we report on the numerical simulation of a harmonic nanocrystal with cubic geometry, pointing out our main results. Finally, in Section IV, we draw some conclusions and outline future perspectives of this work. A brief general description of the basic NNG model is given in the Appendix, together with some computational details.

2 Two-particle simulation: a brief summary of main results

In this Section we summarize the results of a previous simulation, carried out on a simple system of two interacting particles 19. This has been a first but necessary step in demonstrating the ability of the NNG model to reproduce a gravity-induced relaxation towards thermodynamic equilibrium even for a closed system 19.

More specifically we consider the two particles in an harmonic trap, interacting with each other through ‘electrostatic’ and gravitational interaction, whose ‘physical’ Hamiltonian, in the ordinary (first-quantization)
and two-particle von Neumann entropy as a function of time is depicted in Fig. 1 for an initial state of gravitational interactions, with the initial pure state evolving into a mixture \[19\]. The behavior of one-physical Hamiltonian. As a result, we find that entropy fluctuations take place, owing to the (nonunitary part and the corresponding von Neumann entropy is derived as the entanglement entropy with such hidden degrees of freedom. In perspective, the authors would like to add new pieces of evidence on the possible role of gravity in the quantum foundations of thermodynamics in ordinary low-energy physics.

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3 Application to an ideal (harmonic) nanocrystal

The aim of this Section is to go further in the study of nonunitary gravity-induced thermalization, thus in the following we switch to a bit more complex model of a three-dimensional system, that is still computationally tractable. Taking the simple model of an harmonic nanocrystal, in which we consider as in the previous case an artificially augmented gravitational constant, turns out to be a viable choice: indeed the result is a simple and nice formula for thermalization that can be efficiently simulated numerically.
We consider a cubic crystal of volume $V = L^3$. Each phonon propagating within the crystal is supposed to fill it homogeneously, and its gravitational mass is given by $\hbar \omega / c^2$, where $\omega$ is the phonon’s angular frequency. The total Hamiltonian is given by

$$H_G = H_{ph} + H_{hid} + H_{int}$$

where

$$H_{ph} = \sum_{k,s} \hbar \omega_{k,s} \tilde{n}_{k,s} - \frac{1}{4} C(G, V) \sum_{k,s} \sum_{k',s'} \left( \frac{\hbar \omega_{k,s}}{c^2} \right) \left( \frac{\hbar \omega_{k',s'}}{c^2} \right) \tilde{n}_{k,s} \tilde{n}_{k',s'},$$

$$H_{hid} = \sum_{k,s} \hbar \omega_{k,s} \tilde{n}_{k,s} - \frac{1}{4} C(G, V) \sum_{k,s} \sum_{k',s'} \left( \frac{\hbar \omega_{k,s}}{c^2} \right) \left( \frac{\hbar \omega_{k',s'}}{c^2} \right) \tilde{n}_{k,s} \tilde{n}_{k',s'},$$

$$H_{int} = - \frac{1}{2} C(G, V) \sum_{k,s} \sum_{k',s'} \left( \frac{\hbar \omega_{k,s}}{c^2} \right) \left( \frac{\hbar \omega_{k',s'}}{c^2} \right) \tilde{n}_{k,s} \tilde{n}_{k',s'}.$$

Here $\tilde{n}$ and $\tilde{n}$ are, respectively, the physical and hidden phonon number operators. Wave numbers are given by

$$k_i = \frac{2 \pi n_i}{L}, \text{ with } n_i = 0, \pm 1, \pm 2, \ldots \text{ and } -\frac{\pi}{a} < k_i \leq \frac{\pi}{a} \text{ (first Brillouin zone),}$$

while the gravitational factor $C(G, V)$, linearly depending on $G$, is calculated in Appendix B.

We assume a simple dispersion relation, corresponding to a simple cubic crystal structure in which only the first 6 neighbors interaction is taken into account:

$$\omega_{k,s} = \sqrt{\frac{4K}{m}} \sin \left( \frac{ak_s}{2} \right), \quad s = 1, 2, 3$$

where $m$ is the atomic mass, $K$ is the elastic constant and $a$ is the lattice constant.

Indicating by $|n\rangle = |n_{k_1 s_1}, n_{k_2 s_2}, \ldots \rangle$ the state number in the physical Fock space and by $|\tilde{n}\rangle = |\tilde{n}_{k_1 s_1}, \tilde{n}_{k_2 s_2}, \ldots \rangle$ the state number in the hidden Fock space, we note that two generic state numbers $|n\rangle$ and $|\tilde{n}\rangle$ are respectively eigenstates of $H_{ph}$ and $H_{hid}$. This follows from the simple observation that these Hamiltonians depend only on their respective number operators. Let’s call $E_{0,i}$ and $E_{0,j}$ their respective eigenvalues. Now, the product $|n\rangle \otimes |\tilde{n}\rangle$ is an eigenstate of the total Hamiltonian $H_G$ with eigenvalue $E_{0,i} + E_{0,j} + E_{int,i,j}$. As for a really macroscopic (or mesoscopic) body, thermodynamic variables like energy can be defined only at a macroscopic level [20]. In particular, a thermodynamic state with internal energy $E$, at the microscopic level, to specifying energy within an uncertainty $\Delta E$, which includes a huge number of energy levels of the body. For this reason, assuming an initial pure physical state of the form

$$|\psi(0)\rangle = \sum_i \gamma_i |n_i\rangle,$$

where $|n_i\rangle$ are the (physical) energy eigenstates with eigenvalues $E_{0,i}$ close to $E$ (within $\Delta E$), the corresponding meta-state is:

$$||\Psi(0)|| = |\psi(0)\rangle \otimes |\tilde{\psi}(0)\rangle.$$

The state $|\psi(0)\rangle$ is intended to be drawn uniformly at random from the high dimensional subspace corresponding to the energy interval considered. This is reminiscent of the notion of typicality introduced in the context of the Eigenstate Thermalization Hypothesis (ETH) [25], where this concept is more precisely stated by saying that state vector above is distributed according to the Haar measure over the considered subspace [25]. To the purpose of our numerical implementation, the simple algorithm described in Ref. [29] is used.

At time $t$, assuming a complete isolation of the body, we get

$$\|\Psi(t)\| = \sum_{i,j} \gamma_i \gamma_j e^{-(i/h)[E_{0,i} + E_{0,j} + E_{int,i,j}] t} |n_i\rangle \otimes |\tilde{n}_j\rangle \equiv \Gamma_{i,j}(t) |n_i\rangle \otimes |\tilde{n}_j\rangle.$$

The physical state $\rho_{ph}$ is then given by

$$\rho_{ph}(t) = \sum_{i,i'} f_{i,i'}(t) |n_i\rangle \langle n_i'|,$$

with

$$f_{i,i'}(t) = \sum_j \Gamma_{i,j}^+ (t) \Gamma_{i',j} (t) = \gamma_i^* \gamma_{i'} e^{-(i/h)[E_{0,i} - E_{0,i'}] t} \sum_j |\gamma_j|^2 \times \exp \left\{ \frac{i}{2\hbar} C(G, V) \sum_{k,s,k',s'} \left( \frac{\hbar \omega_{k,s}}{c^2} \right) \left( \frac{\hbar \omega_{k',s'}}{c^2} \right) \left[ n_{k,s} - n_{k',s'} \right] n_{k',s'}^t \right\}.$$
This last formula is our central result. In fact the term within the square brackets is the one responsible for the rapid phase cancelation and diagonalization of $\rho_{\text{ph}}(t)$ in the energy basis, as we show in the numerical simulation that follows. Incidentally, we note the strict resemblance of Eq. (15) with Eq. (51) of Ref. [13], expressing the phases cancelation leading to the dynamical self-localization of a lump. This fact reflects the deep connection between the quantum measurement problem and the law of entropy increase, as pointed out in Ref. [20].

In order to perform a simple and viable numerical simulation of the time evolution of the system through the explicit computation of all the terms in Eq. (15), we consider a nanocrystal of $10^3$ atoms, with the following values for the parameters: $m = 3.48 \times 10^{-25} \text{kg}$ (i.e. the mass of $^{210}\text{Po}$, the only chemical element presenting a simple cubic crystal structure), $a = 335 \text{ pm} \ (L = 9a)$ and $K = 23.091 \text{ N/m}$. We put a huge factor $F = 10^{46}$ in front of $G$ in order to simulate the effect of gravity in a really macroscopic system (otherwise the characteristic time of gravitational thermalization for a system of only $10^3$ atoms would be much greater than the age of the Universe!). Besides we choose $E = 1.89 \times 10^{6} \ h\sqrt{K/m}$ and $\Delta E = 0.0024 \ E$.

The numerical calculation of von Neumann entropy amounts to the repeated diagonalization, on a discretized time axis, of the numerical matrix $f_{i,i'}$. Denoting with $\lambda_j$ the eigenvalues of this latter matrix at a given time, von Neumann entropy is readily computed as $S/k_B = -\sum_j \lambda_j \ln \lambda_j$. Its time behaviour is shown in Fig. 2. We can see that the gravitational term at work reproduces correctly the expected behaviour of a thermalizing system. It is expected that the final value of entropy is the maximum value attainable at the given internal energy $E$, provided that the state $\rho_{\text{ph}}$ contains all the available energy eigenstates (given the supposed typicality of the initial state). Since the off-diagonal terms of $\rho_{\text{phys}}$ quickly die out in the basis of the physical energy, consistency with the micro-canonical ensemble, and then with Thermodynamics, is ensured. To be more precise, as it can be immediately seen from Eq. (15), coherences still survive within the degenerate subspaces of energy associated, in the case under study, to a permutation symmetry of the branches $\alpha$. This amounts to a erroneous factor $3!$ in the counting of states, which is practically irrelevant in the computation of entropy due to the huge number of states involved. The characteristic time for entropy stabilization depends of course on the factor $F$ multiplying $G$, that we have inserted to mimic the effect of a really macroscopic crystal. Reducing $F$ amounts to an increase of this time, being the two parameters inversely proportional, thanks to the time-energy uncertainty relation.

![Crystal entropy](image)

Figure 2: Entropy as a function of time for an initial superposition of energy eigenstates within the interval $\Delta E$, showing a monotonic increase and stabilization at late times, as expected for a thermalizing system.

Up to now we have tacitly assumed in our model that the physical and hidden crystals are perfectly superimposed on each other. This circumstance holds true only if a strict CM self-localization is verified, i.e. if our crystal mass is well above the gravitational localization threshold. In the case under study, the big factor $F$ multiplying $G$ has to be taken into account. Localization length can be estimated by using $\Lambda \sim \left( h\sqrt{V/FGM^3} \right)^{1/2} \sim 10^{-15} m \ll L \sim 10^{-9} m$. This latter condition ensures the physical consistency of our calculation.

Finally, let us stress that the present model should be considered just as a toy-model of a real crystal. In fact, in a real crystal the anharmonic corrections play an important role in subsystems’ thermalization, and are of lower order with respect to (nonunitary) gravity, this latter being qualitatively different because of its nonunitary nature. Indeed it is just the nonunitarity which gives rise to the possibility of a net entropy growth.
for the system as a whole, so allowing for a microscopic derivation of the Second Law of thermodynamics. While, of course, the general model need to be tested against properly designed future experiments, anyway we can say that it is the first self-consistent low-energy gravity model implying in a natural way the emergence of Thermodynamics even in a closed system. Incidentally, within the framework of ETH [24, 25], a physical entropy can only be introduced by previously applying an ad-hoc de-phasing map to the state of the system.

4 Conclusions and perspectives

In this work the ability of the NNG model to produce gravity induced thermalization in a closed quantum many-body system has been investigated by studying a specific three-dimensional harmonic nanocrystal model. A numerical simulation compatible with the ETH prescriptions for the choice of the initial state [24, 25] has been carried out, and the time evolution of the system has been calculated. The result shows a monotonic increase of the von Neumann entropy, followed by a stabilization at late times. This behaviour is consistent with that of thermalizing system.

As to the future perspective of this work, the numerical simulation of a more realistic (mesoscopic) crystal is currently under study, in which on the one hand the real value of $G$ is used, and on the other hand the anharmonic terms are explicitly included. These terms are supposed to play an important role to speed up thermalization by letting the phonons interact. They are just the analogue of the electromagnetic interaction acting in the two-particles system discussed in Ref. [19] and recalled in Section 2. It is expected, within this more realistic setting, that even starting from a sharp energy level of the whole crystal, a micro-canonical ensemble would emerge, putting eventually the mechanism of nonunitary gravity-induced thermalization on more robust grounds. If this happens, typicality of the initial state need not to be assumed a priori.

A NNG model: a brief account

In this Appendix we summarize the main features of the NNG model, by focusing on its simplest form, suitably oriented to the problem under study in the main text [8, 9, 10, 12, 13].

Let $H_0[\psi^\dagger, \psi]$ be the non-relativistic ‘physical’ Hamiltonian of a finite number of particle species, like electrons, nuclei, ions and/or molecules, where $\psi^\dagger, \psi$ denote the whole set $\psi^\dagger_i(x), \psi_j(x)$ of creation-annihilation operators, i.e. one couple per particle species and spin component. $H_0[\psi^\dagger, \psi]$ includes the usual electromagnetic interactions accounted for in atomic, molecular and condensed-matter physics.

Let $H_{ph}$ the ‘physical’ energy operator including also the usual Newtonian interaction,

$$H_{ph}[\psi^\dagger, \psi] = H_0[\psi^\dagger, \psi] - \frac{G}{2} \sum_{j,k} m_j m_k \int dx dy \frac{\psi^\dagger_j(x) \psi_j(x) \psi^\dagger_k(y) \psi_k(y)}{|x-y|},$$

(16)

to incorporate that part of gravitational interactions responsible for non-unitality one has to introduce complementary creation-annihilation operators $\tilde{\psi}^\dagger(x)$, $\tilde{\psi}(x)$ and the overall (meta-)Hamiltonian:

$$\mathcal{H}_{TOT} = H_{ph}[\psi^\dagger, \psi] + H_{hid}[\tilde{\psi}^\dagger, \tilde{\psi}]$$

$$- \frac{G}{4} \sum_{j,k} m_j m_k \int dx dy \left[ \frac{2\psi^\dagger_j(x) \psi_j(x) \tilde{\psi}^\dagger_k(y) \tilde{\psi}_k(y)}{|x-y|} \right]$$

$$+ \frac{G}{4} \sum_{j,k} m_j m_k \int dx dy \left[ \frac{\psi^\dagger_j(x) \psi_j(x) \tilde{\psi}^\dagger_k(y) \tilde{\psi}_k(y)}{|x-y|} \right]$$

$$+ \frac{G}{4} \sum_{j,k} m_j m_k \int dx dy \left[ \frac{\tilde{\psi}^\dagger_j(x) \tilde{\psi}_j(x) \tilde{\psi}^\dagger_k(y) \tilde{\psi}_k(y)}{|x-y|} \right].$$

(17)

The above operators act on the product $F_\psi \otimes F_{\tilde{\psi}}$ of Fock spaces of the $\psi$ and $\tilde{\psi}$ operators, where $m_i$ is the mass of the $i$-th particle species and $G$ is the gravitational constant. The $\tilde{\psi}$ operators obey the same statistics as the corresponding operators $\psi$, while $[\psi, \tilde{\psi}] = [\psi, \tilde{\psi}] = 0$.

The meta-particle state space $S$ is the subspace of $F_\psi \otimes F_{\tilde{\psi}}$, including the meta-states obtained from the vacuum $|0\rangle = |0\rangle_\psi \otimes |0\rangle_{\tilde{\psi}}$ by applying operators built in terms of the products $\psi^\dagger_j(x) \tilde{\psi}^\dagger_j(y)$ and symmetrical with respect to the interchange $\psi^\dagger \leftrightarrow \tilde{\psi}^\dagger$; as a consequence they have the same number of $\psi$ (physical) and $\tilde{\psi}$ (hidden) meta-particles of each species. Since constrained meta-states cannot distinguish between physical and hidden operators, the observable algebra is identified with the physical operator algebra. In view of this,
expectation values can be evaluated by preliminarily tracing out the $\bar{\psi}$ operators. In particular, the most general meta-state corresponding to one particle states is represented by

$$\langle |f\rangle = \int dx \int dy f(x,y)\psi_j^\dagger(x)\bar{\psi}_j(y) |0\rangle,$$

with

$$f(x,y) = f(y,x).$$

This is a consistent definition since $\mathcal{H}_{TOT}$ generates a group of (unitary) endomorphisms of $S$.

Note that $\mathcal{H}_{TOT}$ and $\mathcal{H}_{ph}[\psi^\dagger,\psi] + \mathcal{H}_{hid}[\bar{\psi}^\dagger,\bar{\psi}]$ differ only due to correlations. In fact, because of the state constraint, the hidden degrees of freedom show the same average energy of the observed ones, while the two last sums in $\mathcal{H}_{TOT}$ have approximately equal expectation values and fluctuate around the classical gravitational energy. These fluctuations, though irrelevant on a macroscopic scale, are precisely what can lead to thermodynamic equilibrium in a closed system if thermodynamic entropy is identified with von Neumann entropy [3].

**B Calculation of $C(G,V)$**

Let’s calculate the gravitational interaction between two phonons, supposed to fill homogeneously the crystal of cubic form. Their mass are expressed by

$$m_i = \frac{\hbar \omega_k}{c^2}, \quad i = 1,2$$

while their gravitational interaction energy is

$$U_G = -m_1 m_2 C(G,V) = -m_1 m_2 G V^{-1/3} \Im,$$

where

$$\Im = \int_0^1 d\xi \int_0^1 d\eta \int_0^1 d\zeta \int_0^1 d\xi' \int_0^1 d\eta' \int_0^1 d\zeta' \frac{1}{\sqrt{(\xi - \xi')^2 + (\eta - \eta')^2 + (\zeta - \zeta')^2}} \simeq 1.87.$$ (21)

This value has been obtained by means of two different numerical methods with the software @Mathematica.

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