Entanglement energetics in the ground state

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Abstract

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Entanglement Energetics in the Ground State

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We show how many-body ground state entanglement information may be extracted from subsystem energy measurements at zero temperature. A precise relation between entanglement and energy fluctuations is demonstrated in the weak coupling limit. Examples are given with the two-state system and the harmonic oscillator, and energy probability distributions are calculated. Comparisons made with recent qubit experiments show this type of measurement provides another method to quantify entanglement with the environment.

A standard assumption in thermodynamics is that the coupling energy of the system to the thermodynamic bath must be smaller than any other energy scale in the problem. In this paper, we explore the consequences of the violation of this assumption when the combined system and bath are together in the overall ground state (or at zero temperature). From the thermodynamic point of view, this is a boring situation because nothing can happen: the system and bath cannot exchange energy. However, from a quantum mechanical point of view, the non-vanishing of the coupling energy can play an important role for mesoscopic systems (where the thermodynamic limit cannot be applied). Thermodynamic relations must be applied only to the entire system. In fact, even though the system is at zero temperature, if a measurement of a sub-system Hamiltonian is made, it can be found in an excited state with a probability that depends on the coupling to its environment. This non-intuitive result is a purely quantum phenomenon: it is a consequence of entanglement of the sub-system with the environment. In fact, we demonstrate that knowledge of the probability to find the system in an excited state can be used to determine the degree of entanglement of the sub-system and bath. Consequently, simple systems with well known isolated quantum mechanical properties (such as the two-state system and harmonic oscillator) become “entanglement-meters”.

There is growing interest in ground-state entanglement from the condensed matter physics community. Theoretical works on ground state entanglement have addressed entropy scaling in harmonic networks, spin-spin entanglement in quantum spin chains, and quantum phase transitions. Entanglement properties of the ground state are also essential in the field of adiabatic quantum computing. Recently, there has also been interest in the relationship between energy frustration and entanglement. It is also interesting to link other ground state properties of a variety of mesoscopic systems to the zero-temperature entanglement energetics. These properties include the persistent current of small mesoscopic rings or of doubly connected Cooper pair boxes, single Cooper pair boxes measured by a dc-SQUID, and the occupation of resonant states. Furthermore, the role of entanglement with an unmonitored environment in the decoherence of scattering quantum particles has been considered for many-body quantum chaotic baths and recently at zero temperature.

It has long been recognized that the ground state properties of mesoscopic systems are very interesting. In particular, a small metallic loop penetrated by an Aharonov-Bohm flux exhibits a persistent current if the temperature is so low that the phase coherence length becomes larger than the circumference. It is therefore of interest to investigate the persistent current in rings coupled to a bath. The ground state of a model of a ring with a quantum dot coupled capacitively to a resistor was examined by Cedraschi et al. and it was found that the persistent current decreases with increasing coupling strength and at the same time that the persistent current is not sharp but fluctuates with a variance that increases with increasing coupling strength. To explain these results these authors already alluded to energy fluctuations. Such an explanation implies a close connection between energy fluctuations and persistent current fluctuations. Indeed in the work presented here we substantiate this relationship. A simple and transparent model in which energy fluctuations can be investigated is that of an oscillator coupled to a bath of harmonic oscillators. Nagaev and one of the authors calculated the variance of the energy of the oscillator as a function of the coupling strength to the bath. In the work presented here, we analyze not only the variance but the entire distribution function of energy of the oscillator in its ground state, and show how these fluctuations originate from entanglement.

We consider a general Hamiltonian $H = H_s + H_c + H_E$, that couples ($c$) the system ($s$) we are interested in to a quantum environment ($E$) such as a network of harmonic oscillators. The lowest energy separable state is $|S⟩ = |0⟩_s |0⟩_E$, where $|0⟩_s$ is the lowest uncoupled energy state of both systems. However, if the system Hamiltonian and the total Hamiltonian do not commute (which is the generic situation), then $|S⟩$ is not an energy eigenstate of the total Hamiltonian. Thus, there must be a lower energy eigenstate ($|0⟩$) of the total Hamiltonian which is by definition an entangled state. Because time evolution is governed by the full Hamiltonian, the ground state expectation of any operator with no explicit time dependence will have no time evolution, insuring that any measurement outcome is static in time. This situation is in contrast to the usual starting point of assuming that the initial state is a separable state and studying how it becomes entangled. The reduced density operator of the system is given by tracing out the environmental degrees of freedom, $ρ = Tr_E |0⟩⟨0|$. Assuming the full state of the whole
system is pure, the reduced density matrix contains all accessible system information, including entanglement of the system with its environment. Because repeated measurements of $H_s$ will give different energies as the sub-system is not in an energy eigenstate, we are interested in a complete description of the statistical energy fluctuations. These fluctuations may be described in two equivalent ways. The first way is to find the diagonal density matrix elements in the basis where $H_s$ is diagonal. These elements represent the probability to measure a particular excited state of $H_s$. A second way is to find all energy cumulants. A cumulant of arbitrary order may be calculated from the sub-system energy generating function, $Z(\chi) = \langle \exp(-\chi H_s) \rangle$ (as always, $\langle O \rangle = \text{Tr} \rho O$) so that the $n^{th}$ energy cumulant is given by

$$\langle \langle H_s^n \rangle \rangle = (-)^n \frac{d^n}{d\chi^n} \ln Z(\chi) \bigg|_{\chi=0}. \quad (1)$$

These cumulants give information about the measured energy distribution around the average.

Before proceeding to calculate these energy fluctuations, we ask a general question about entanglement. Given the energy distribution function (the diagonal matrix elements of the density matrix only), can anything be said in general about the purity or entropy of the state? Surprisingly, because we are given the additional information that we are at zero temperature, the answer is yes. If we ever measure the sub-system’s energy and find an excited energy, then we know the state is entangled. Although this statement alone links energy fluctuations with entanglement, a further quantitative statement may be made in the weak coupling limit. The reason for this is the following: the assumptions exponentially suppress higher states, so to first order in the coupling constant, we can consider a two-state system where the density matrix has the form

$$\rho = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \alpha \begin{pmatrix} -p & c \\ c^* & p \end{pmatrix} + \mathcal{O}(\alpha^2). \quad (2)$$

For vanishing coupling constant $\alpha = 0$, the first term is just the density matrix for the separable state. The linear dependence of $\rho$ on $\alpha$ holds to first order for the model systems considered below and is the entanglement contribution. If one measures the diagonal elements of $\rho$, one obtains $p_{\text{down}} = 1 - p\alpha$ and $p_{\text{up}} = p\alpha$ as the probability to be measured in the ground or excited state (because $\alpha$ is small, there is only a small probability to find the sub-system in the upper state). If we now diagonalize $\rho$, the eigenvalues are $\lambda_{1,2} = \{1 - p\alpha, p\alpha\} + \mathcal{O}(\alpha^2)$. To first order in $\alpha$, the eigenvalues are the diagonal matrix elements, so we may (to a good approximation) write the purity or entropy in terms of these probabilities even if the energy difference remains unknown.

The Qubit. Let us now first evaluate the energy fluctuations of a qubit, a two-state system. The most general (trace 1) spin density matrix is $\rho = (\mathbb{1} + \langle \sigma_x \rangle \sigma_x + \langle \sigma_y \rangle \sigma_y + \langle \sigma_z \rangle \sigma_z)/2$. A simple measure of the entanglement is given by the purity. $\text{Tr} \rho^2 = (1/2)(1 + X^2 + Y^2 + Z^2)$, where $X_i = \langle \sigma_i \rangle$. It is well known that $(X, Y, Z)$ form coordinates in the Bloch sphere. Purity lies at the surface where $X^2 + Y^2 + Z^2 = 1$, whereas corruption lies deep in the middle.

We take the system Hamiltonian\textsuperscript{25} to be $H_s = (\epsilon/2) \sigma_z + (\Delta/2) \sigma_x$. Introducing the frequency $\Omega = \sqrt{\epsilon^2 + \Delta^2}/\hbar$ and using the identity $e^{-i\frac{\Delta}{\hbar}\sigma_z} = I \cos \frac{\Delta}{2} - i\hat{n} \cdot \hat{\sigma} \sin \frac{\Delta}{2}$ with $\beta = \hbar\chi\Omega$, and the unit vector $\hat{n}$ chosen to give $e^{-i\chi H_s}$
for the general case, we use a perturbative solution which is only valid for large $\epsilon$ or large $\alpha$. After Ref. 1.

\[(n_z = \epsilon/h\Omega, n_x = \Delta/h\Omega),\] it is straightforward to show

\[Z(i\chi) = \cos(h\Omega\chi/2) - \sin(h\Omega\chi/2)\] \[\frac{\sin(\hbar\Omega\chi/2)}{\hbar\Omega}(\langle \sigma_z \rangle + \Delta \langle \sigma_z \rangle).\] (3)

The energy probability distribution may be easily found by Fourier transforming Eq. (3), or by tracing in the diagonal basis of the system Hamiltonian. The answer may be expressed with only the average energy, $\langle H_s \rangle = \sigma_z/2 + \sigma_z/2$, as a sum of delta functions at the system energies $\pm \hbar\Omega/2$ with weights of the diagonal density matrix elements,

\[\langle \delta(E - H_s) \rangle = \frac{\delta(E + \hbar\Omega/2)}{2} \left[ 1 - \frac{\langle H_s \rangle}{\hbar\Omega/2} \right] + \frac{\delta(E - \hbar\Omega/2)}{2} \left[ 1 + \frac{\langle H_s \rangle}{\hbar\Omega/2} \right].\] (4)

Clearly, if the spin is isolated from the environment, $\langle H_s \rangle = -\hbar\Omega/2$ (the ground state energy), the probability weight to be in an excited state vanishes. This distribution may also be found from knowledge of the isolated eigenenergies, the fact that $\langle H_s \rangle = \sum_j E_j \rho_{jj}$, and that $\text{Tr} \rho = 1$. This later argument may be extended to n-state systems given the first $n - 1$ moments of the Hamiltonian and the n eigenenergies.

Connection with Real Qubits. The probability weights depend on the energy parameters $\epsilon$ and $\Delta$, and the expectation values of the Pauli matrices. For real qubits produced in the lab, these will depend on the environment. Often, we can link the basic phenomena we have been describing to physical measurements other than energy. Consider, for example, a mesoscopic ring threaded by an Aharonov-Bohm flux $\Phi$ shown in Fig. 1. The ring has an in-line quantum dot coupled to it with tunneling contacts, where the tunneling matrix elements $t_L, t_R$ depend on the flux $\Phi$. Interactions between the ring and dot are described with the capacitances $C_L$ and $C_R$. The dot-ring structure is capacitively coupled to an external impedance $Z_{ext}$ modeled by an infinite chain of LC-oscillators. This external impedance plays the role of the quantum environment. The equilibrium state of the dot-ring system supports a persistent current as a function of flux. The persistent current is related to the effective two-level system operators only, and in turn may be related to the probability to find the excited energy state for the symmetric case of $\epsilon = 0$,

\[p_{up} = \frac{1}{2} \left[ 1 + \frac{\langle H_s \rangle}{\hbar\Omega/2} \right] = \frac{1}{2} \left[ 1 - \frac{I(\Phi)}{I_0(\Phi)} \right].\] (5)

where $I_0(\Phi)$ is the uncoupled value of the persistent current. This physical implementation gives a direct translation between the measured persistent current and the entanglement between ring and dot. Different discussions of the effect of a bath on persistent current should be classified as whether the system Hamiltonian commutes with the total Hamiltonian (see Ref. 13) or does not (see Refs. 11,12). Another physical system that shows similar physics is a quantum dot connected in series with a tunnel junction, metallic reservoir and quantum impedance represented by a bosonic environment.

A common model for environmental effects is given by coupling the two-state system to a series of harmonic oscillators, the spin-boson model. In Fig. 2 we have plotted the upper and lower occupation probabilities for the spin-boson model as a function of the coupling constant $\alpha$. For the symmetric case ($\epsilon = 0$), we have used the
The ansatz solution\textsuperscript{11,28}, while for $\epsilon$ finite, we have used the perturbative solution in $\Delta/\omega_c$, which is valid only for larger $\alpha$ or $\epsilon$.\textsuperscript{11} Thus the plot is cut off at a small $\alpha$. A computational approach calculating the expectation values of the Pauli matrices over the whole parameter range was given in Ref.\textsuperscript{26}. The quantum dynamics of this system was studied in Ref.\textsuperscript{24}. One simple measure of the bath type is the slope of the occupation probability in the vicinity of $\alpha = 0$.

Experiments are always carried out at finite temperature, and it is important to demonstrate that there exists a cross-over temperature to the quantum behavior discussed here. For an isolated system in thermal equilibrium, where the coupling energy plays no role, the (low-temperature) thermal occupation probability is $p_{th} = \exp[-(E_2 - E_1)/kT]$. In the weak coupling limit for the symmetric spin boson problem, the probability to measure the excited state scales as $p_{up} = -\alpha \log(\Delta/\omega_c)$.\textsuperscript{30} Setting these factors equal and solving for $T^*$ yields

$$kT^* = \frac{E_2 - E_1}{\log(\alpha \log \frac{\Delta}{\omega_c})}. \quad (6)$$

Since $T^*$ scales as the inverse logarithm of the coupling constant, it is experimentally possible to reach a regime where thermal excitation is negligible. If one carefully calculates many-body low temperature corrections to the zero temperature results, one obtain corrections quadratic in temperature.\textsuperscript{32} As an order of magnitude estimate, we compare with the Cooper pair box which is among the most environmentally isolated solid state qubits.\textsuperscript{14} From which found a $Q \sim 10^4$, we estimate the quantum probability for the box to be measured in the excited state as $p_{up} \sim 10^{-3} - 10^{-4}$, which is of same order or larger than the thermal probability, $p_{th} \sim 10^{-4}$. Experimentally, $p_{up}$ and $p_{th}$ may be confused by fitting data with an effective temperature, $p_{th} \propto \exp(-\beta_{eff} H_s)$.\textsuperscript{33} However, one may distinguish true thermal behavior from the effect described here because $p_{up}$ and $p_{th}$ depend differently on tunable system parameters such as $\Delta$. In fact, $\beta_{eff}$ is an entanglement measure. The behavior discussed here is closely related to the breakdown of the concept of local temperature discussed in Ref.\textsuperscript{32}

\textbf{The Harmonic Oscillator.} We now consider the entanglement energetics of a harmonic oscillator, $H_s = p^2/(2m) + (1/2)m\omega^2q^2$. Since there are an infinite number of states, the problem is harder. To simplify our task, we assume a linear coupling with an harmonic oscillator bath. This implies that the density matrix is Gaussian so that environmental information is contained in the second moments $\langle q^2 \rangle$ and $\langle p^2 \rangle$.\textsuperscript{23}

$$\langle q|\rho|q' \rangle = \frac{1}{\sqrt{2\pi \langle q^2 \rangle}} \exp\left\{ -\frac{(q-q')^2}{2\langle q^2 \rangle} - \frac{(p^2)(q-q')^2}{2\hbar^2} \right\}. \quad (7)$$

Expectation values of higher powers of $H_s$ are non-trivial because $q$ and $p$ do not commute. The purity of the density matrix Eq. (7) is

$$\text{Tr}\rho^2 = \int dq dq' \langle q|\rho|q' \rangle \langle q'|\rho|q \rangle = \frac{\hbar/2}{\sqrt{\langle q^2 \rangle \langle p^2 \rangle}}. \quad (8)$$

The uncertainty relation, $\sqrt{\langle q^2 \rangle \langle p^2 \rangle} \geq \hbar/2$, guarantees that $\text{Tr}\rho^2 \leq 1$, with the inequality becoming sharp if the oscillator is isolated from the environment. As the environment causes greater deviation from the Planck scale limit, the state loses purity.

The generating function $Z$ may be calculated conveniently by tracing in the position basis and inserting a complete set of position states between the operators,

$$Z(\chi) = \int dq dq' \langle q|\rho|q' \rangle \langle q'|e^{-\chi H_s}|q \rangle. \quad (9)$$

The first object in Eq. (9) is the density matrix in position representation, given by Eq. (7). The second object may be interpreted as the uncoupled position-space propagator of the harmonic oscillator from position $q$ to $q'$ in time $-i\hbar\chi$,

$$\langle q'|e^{-\chi H_s}|q \rangle = \left[ \frac{m\omega}{2\pi \hbar \sinh \hbar \omega \chi} \right]^{1/2} \exp\left\{ -\frac{m\omega}{2\hbar \sinh \hbar \omega \chi} [(q^2 + q'^2) \cosh \hbar \omega \chi - 2qq'] \right\}. \quad (10)$$

This interpretation is quite general and may be used to extend this analysis to other systems. We find

$$Z(\chi) = \left\{ 2E_s \frac{\sinh \varepsilon \chi}{\varepsilon} + 2A (\cosh \varepsilon \chi - 1) + \frac{1 + \cosh \varepsilon \chi}{2} \right\}^{-\frac{1}{2}}. \quad (11)$$
where $\varepsilon = \hbar \omega$, $2E = m \omega^2 (q^2) + (p^2)/m$ and $A = \langle q^2 \rangle \langle p^2 \rangle / \hbar^2$. $E$ is the average energy of the oscillator, while $A \geq 1$ is a measure of satisfaction of the uncertainty principle. Eq. (11) has a pleasing limit for the free particle $\omega \to 0$,

$$Z(\chi)_{\text{free}} = \left\{ 1 + \chi \langle p^2 \rangle / m \right\}^{-\frac{1}{2}},$$

which is just the generating function for Wick contractions, $\langle p^2n \rangle = (2n - 1)!! \langle \langle p^2 \rangle \rangle^n$. Thus, in Eq. (11), the inverse square root generates the right combinatorial factors under differentiation, and the nontrivial $\chi$ dependence accounts for the commutation relations between $q$ and $p$. The first few harmonic oscillator energy cumulants may now be straightforwardly found via Eq. (11),

$$\langle H^2 \rangle = (1/2)[-\langle \varepsilon^2 / 2 \rangle + 4E^2 - 2\varepsilon^2 A],$$

$$\langle H^4 \rangle = -(E/2)[-16E^2 + \varepsilon^2 (1 + 12A)],$$

$$\langle H^6 \rangle = 48E^4 - 4\varepsilon^2E^2(1 + 12A) + \varepsilon^4 [(1/8) + 2A + 6A^2].$$

After inserting the mean square values for an ohmic bath (see the discussion above eqs. (21,22)), Eq. (13) is identical to the main result of Nagaev and one of the authors.

Alternatively, we now consider the diagonal matrix elements $\rho_{nm}$. An analytical expression for the density matrix in the energy basis may be found by using the wavefunctions of the harmonic oscillator,

$$\psi_n(q) = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} e^{-\gamma q^2 / 2} H_n(\gamma q)$$

where $\gamma = \sqrt{m \omega / \hbar}$ and $H_n(x)$ is the $n^{th}$ Hermite polynomial. In the energy basis, the density matrix is given by $\rho_{nm} = \int dq dq' \psi^*_n(q) \langle q | \rho | q' \rangle \psi_m(q')$. The position space integrals may be done using two different copies of the generating function for the Hermite polynomials.

$$G(q, s) = e^{-s^2 + 2xs} = \sum_{m=0}^{\infty} \frac{H_m(q) s^m}{m!}.$$  

The diagonal elements may be found by equating equal powers of the generating variables. We first define the dimensionless variables $x = 2 \gamma^2 \langle q^2 \rangle$, $y = 2 \langle p^2 \rangle / (\gamma^2 \hbar^2)$, and $D = 1 + x + y + xy$. $x$ and $y$ are related to the major and minor axes of an uncertainty ellipse. The isolated harmonic oscillator (in its ground state) obeys two important properties: minimum uncertainty (in position and momentum) and equipartition of energy between average kinetic and potential energies. The influence of the environment causes deviations from these ideal behaviors which may be accounted for by introducing two new parameters, $a = (y - x)/D$, $b = (xy - 1)/D$ with $-1 \leq a \leq 1$ and $0 \leq b \leq 1$. The deviation from equipartition of energy is measured by $a$, while the deviation from the ideal uncertainty relation is measured by $b$. We find

$$\rho_{nn} = \frac{4}{D} \left( b^2 - a^2 \right)^{n/2} P_n \left[ b / \sqrt{b^2 - a^2} \right],$$

where $P_n[z]$ are the Legendre polynomials. The first few energy probabilities are given below (without the $\sqrt{4/D}$ prefactor).

<table>
<thead>
<tr>
<th>$n$</th>
<th>$\rho_{nn}/\rho_{00}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>$b$</td>
</tr>
<tr>
<td>2</td>
<td>$a^2/2 + b^2$</td>
</tr>
<tr>
<td>3</td>
<td>$3a^2b/2 + b^3$</td>
</tr>
<tr>
<td>4</td>
<td>$3a^4/8 + 3a^2b^2 + b^4$</td>
</tr>
<tr>
<td>5</td>
<td>$15a^4b/8 + 5a^2b^3 + b^5$</td>
</tr>
<tr>
<td>6</td>
<td>$5a^6/16 + 45a^4b^2/8 + 15a^2b^4/2 + b^6$</td>
</tr>
<tr>
<td>7</td>
<td>$35a^6b/16 + 105a^4b^3/8 + 21a^2b^5/2 + b^7$</td>
</tr>
</tbody>
</table>

If we try and choose $x$ and $y$ so as to violate the uncertainty principle, unphysical results appear as some of the probabilities exceed 1, or become negative. The probabilities also reveal environmental information. For example, $\rho_{11}/\rho_{00} = b$ and is thus only sensitive to the area of the state, while $\rho_{22}/\rho_{00} = a^2/2 + b^2$ depends on both the
uncertainty and energy asymmetry. Additionally, if we expand the first density matrix eigenvalue\(^{23}\) with respect to small deviations of \(x\) and \(y\), we recover \(\rho_{11}\) in agreement with our general argument. To complete the circle, we may make an “energy transform” on these probabilities,

\[
Z(\chi) = \sum_{n=0}^{\infty} e^{-\chi E_n} \rho_{nn},
\]

where \(E_n = (n + 1/2)\hbar \omega\) are the uncoupled energy eigenvalues of the harmonic oscillator. If we now identify the new generating variable \(t = \sqrt{b^2 - a^2} \exp(-\chi \hbar \omega)\) and deviation variable \(z = b/\sqrt{b^2 - a^2}\), we may make use of the summation formula for the Legendre polynomials\(^{33}\)

\[
\sum_{n=0}^{\infty} t^n P_n[z] = \left(1 - 2zt + t^2\right)^{-1/2},
\]

to recover (after some algebra) the energy generating function Eq. (11).

Although \(x\) and \(y\) have been treated as independent variables, the kind of environment the system is coupled to replaces these variables with two functions of the coupling constant. For example, with the ohmic bath\(^{33}\) (in the under-damped limit), the variables are

\[
\begin{align*}
x(\alpha) &= \frac{1}{\sqrt{1 - \alpha^2}} \left(1 - \frac{2}{\pi} \arctan\frac{\alpha}{\sqrt{1 - \alpha^2}}\right), \\
y(\alpha) &= (1 - 2\alpha^2)x(\alpha) + \frac{4\alpha}{\pi} \ln\frac{\omega_c}{\omega},
\end{align*}
\]

where \(\alpha\) is the coupling to the environment in units of the oscillator frequency and \(\omega_c\) is a high frequency cutoff.

This bath information is shown in Fig. 3 with \(\omega_c = 10\omega\). The trajectory of the line over the surface shows how the probabilities evolve as the coupling \(\alpha\) is increased from 0 to 1. Other kinds of environments would trace out different contours on the probability surface.

In conclusion, we have shown that projective measurements of the system Hamiltonian at zero temperature reveal entanglement properties of the many-body quantum mechanical ground state. Consequently, repeated experiments
on simple quantum systems give information about the nature of the environment, the strength of the coupling and entanglement. The larger the energy fluctuations, the greater the entanglement. There are several possibilities for experimental implementations. We have mentioned measurement of persistent current\textsuperscript{11,12,13} as well as projecting on the system’s energy eigenstates. Another measurement possibility is a zero temperature activation-like process\textsuperscript{34} where the dominant mechanism is not tunneling, but the same quantum effects of the environment which we have discussed here.

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