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Effective localization induced by noise and nonlinearity

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Abstract

With the aid of a very simple model with only two possible configurations, we study the dynamical transition from delocalized to localized states for quantum bistable systems. Results may have relevance for the understanding of the phenomenology of some mesoscopic systems which are usually found in a localized state as for example pyramidal AsH_3 molecule. The interaction with the environment is modeled by considering both external noise disturbance and nonlinear effects due to the contraction of the Hilbert space. The noise alone produces decoherence and suppression of tunneling, but delocalized states spontaneously evolve into localized ones only when nonlinearity is also present.

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1. Introduction

In this paper, we propose a model for the evolution of bistable quantum systems into a localized state. It turns out, in fact, that at low temperature, systems with a symmetric potential are found to be localized in one of the two minima.

A typical example is a class of pyramidal molecule as for example AsH_3 (see [1] and reference cited therein), whose symmetry implies two specular minima. The problem is puzzling since in the absence of perturbations of any kind, one would expect to find the system in a delocalized ground state at low temperature, while empirical evidence is for asymmetric localization.

From an equilibrium point of view, an answer was already given. In fact, systems with bistable potentials are very sensitive to perturbations [1]. If some semi-classical conditions are verified, the symmetry can be easily broken by an extremely small disturbance and a localized ground state emerges.

In this paper, we focus our attention on dynamics, in fact, the equilibrium description does not explain how the localization is reached. In other words, if the two minima of the potential correspond to localized states with a minimal energy gap, coherent tunneling between them is allowed except for a vanishing temperature.

It is well known that environment induces decoherence (see for example [2–6]) and this fact could

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explain why coherent tunneling is dumped. Nevertheless, the fundamental problem remains, how it happens that a delocalized individual system evolves into a localized state?

We try to give an answer by considering ab initio a two configurations model. In Section 2, we introduce a linear toy system, whose time independent Hamiltonian is simply represented by a spin in a constant magnetic field. At this level, noise is absent and the system tunnels coherently and periodically.

Then, in Section 3 we consider the effect of a time dependent perturbation (interaction with the environment). This perturbation is modelized by a stochastic magnetic field perpendicular to the original one. Now, the off-diagonal terms of the averaged density matrix disappear for large times, i.e. there is decoherence. Furthermore, for strong noise, there is suppression of tunneling, which means that a system initially localized persists in its stable configuration (see also [7–9]). Nevertheless, a system, which is not in a localized state, does not spontaneously evolve into a localized one. From a mathematical point of view, this means that while the averaged density matrix becomes diagonal in the limit of large times, this is not the case for the density matrix associated to a single realization of the noise.

We then consider the same model, but we assume that the constant magnetic field is replaced by a nonlinear interaction. In the absence of perturbations (Section 4), it turns out that the system behaves qualitatively as in the linear unperturbed case of Section 2. But, by this fall, if the same stochastic perturbation of Section 3 is introduced (Section 5), one finds that after a transient, the system is most of the time in one of the two localized states. From a mathematical point of view, this means that not only the averaged matrix is diagonal, but the matrix associated to a single realization of the noise is most of the time very close to

$$\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

or to

$$\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

Quick transitions between the two stable configurations are always possible, but their frequency vanishes for large times. In this sense, we speak of effective localization. The conclusion is that both nonlinearity and noise are fundamental ingredients for spontaneous evolution in localized states.

2. Linear model in the absence of noise

Hamiltonian of a bistable system can be written down in terms of Pauli matrices and the density matrix of a state can be written in a convenient form using the vector $\mathbf{x} = (x, y, z)$ defined by

$$\rho = \frac{1}{2}\begin{pmatrix} 1+z & x-\mathrm{i}y \\ x+\mathrm{i}y & 1-z \end{pmatrix}. \tag{1}$$

The trace of this density operator equals 1 (normalization) and the determinant vanishes for a pure state. This last requirement implies $|\mathbf{x}| = 1$ (a pure state is represented by a point on the unitary sphere).

The third component z of this vector encodes the information about the localization ($z = \pm 1$ means that the system is exactly localized in one of the two states), while x and y encode the information about coherence (when they vanish, there is complete decoherence).

The above considerations show that the quantum evolution $\dot{\rho} = -\mathrm{i}[H, \rho]$ corresponds to the motion of a point on a unitary sphere. When the point is in one of the two poles, the system is localized.

Hamiltonian, which describes an isolated two configurations system, allowed for tunneling is typically

$$H = \alpha\sigma_x, \tag{2}$$

where σ_x is the Pauli matrix. This Hamiltonian produces coherent quantum tunneling of period π/α between the two *macroscopic* configurations of the system (in mathematical terms, the two eigenstates of the Pauli matrix σ_z).

The corresponding equations for $\mathbf{x}$ are

$$\dot{x} = 0, \qquad \dot{y} = -2\alpha z, \qquad \dot{z} = 2\alpha y. \tag{3}$$

It is clear that (2) induces a rotation with constant angular velocity around the x-axis. The value of the first component of the vector remains unchanged. Therefore, (2) never allows for localization or decoherence.

3. Linear model: decoherence induced by noise

Assume now that the interaction with the environment is described by

$$H = \alpha\sigma_x + \epsilon(t)\sigma_z, \tag{4}$$

where σ_x and σ_z are Pauli matrices and $\epsilon(t)$ is a given realization of a stochastic process. The presence of a nonvanishing $\epsilon(t)$ means that we introduce an interaction with the environment which randomly breaks in time the energy symmetry of the two configurations.

We find that the vector $\mathbf{x}$ satisfies

$$\dot{x} = -2\epsilon(t)y, \qquad \dot{y} = +2\epsilon(t)x - 2\alpha z, \\ \dot{z} = +2\alpha y, \tag{5}$$

which is the superposition of two rotations, the first around the x-axis with constant angular velocity 2α, the second around the z-axis with time dependent angular velocity $2\epsilon(t)$.

Assume $\epsilon(t) = \beta\eta(t)$, where $\eta(t)$ is a given realization of a white noise (i.e. $w(t) \equiv \int_0^t \eta(s)\,\mathrm{d}s$ is a Brownian motion). In Stratanovitch notation the only thing we have to do is to substitute $\epsilon(t)$ with $\beta\eta(t)$ in the above equations. Nevertheless, it is much more practical to use Ito notation for which Eq. (5) is written as

$$\mathrm{d}x = -2\beta^2 x\,\mathrm{d}t - 2\beta y\,\mathrm{d}w, \\ \mathrm{d}y = -2\beta^2 y\,\mathrm{d}t - 2\alpha z\,\mathrm{d}t + 2\beta x\,\mathrm{d}w, \\ \mathrm{d}z = +2\alpha y\,\mathrm{d}t. \tag{6}$$

From (6), taking the expectation value, we immediately obtain

$$\dot{\bar{x}} = -2\beta^2\bar{x}, \qquad \dot{\bar{y}} = -2\beta^2\bar{y} - 2\alpha\bar{z}, \\ \dot{\bar{z}} = +2\alpha\bar{y}. \tag{7}$$

Since the density matrix depends linearly on $\mathbf{x}$, the above equation describes the evolution of the averaged density matrix $\bar{\rho}$. This matrix describes the mixture of all the states associated to the ensemble of all the realizations of the noise in the Hamiltonian (4). In other words, if one cannot know which is the noise realization, all the statistical provisions are those that can be derived from the averaged density matrix $\bar{\rho}$.

Eq. (7) can be easily solved. When $\beta^2 < 2|\alpha|$, the solution is

$$\overline{x(t)} = \mathrm{e}^{-2\beta^2 t}x(0), \\ \overline{y(t)} = \mathrm{e}^{-\beta^2 t}[y(0)\cos(\omega t) + c_1\sin(\omega t)], \\ \overline{z(t)} = \mathrm{e}^{-\beta^2 t}[z(0)\cos(\omega t) + c_2\sin(\omega t)], \tag{8}$$

where $\omega = \sqrt{|\beta^4 - 4\alpha^2|}$, $c_1 = (-\beta^2 y(0) - 2\alpha z(0))/\omega$ and $c_2 = (\beta^2 z(0) + 2\alpha y(0))/\omega$. Looking at the third component $z(t)$, one realizes that in this region a quantum coherent behavior partially survives to the noise for a certain time.

When $\beta^2 > 2|\alpha|$, the solution is purely exponential and is given by

$$\overline{x(t)} = \mathrm{e}^{-2\beta^2 t}x(0), \\ \overline{y(t)} = \mathrm{e}^{-\beta^2 t}[y(0)\cosh(\omega t) + c_1\sinh(\omega t)], \\ \overline{z(t)} = \mathrm{e}^{-\beta^2 t}[z(0)\cosh(\omega t) + c_2\sinh(\omega t)]. \tag{9}$$

In this strong noise region the coherent behavior is completely destroyed since the localization probability relaxes exponentially. The interesting fact is that for large β, $\overline{z(t)}$ relaxes with an exponent which vanishes as $2\alpha^2/\beta^2$. This fact means that the time necessary for delocalization becomes infinite in the limit of extremely strong noise.

Summarizing, we have damped oscillations for a weak interaction with the environment ($\beta^2 < 2|\alpha|$) and incoherent relaxation for strong interaction ($\beta^2 > 2|\alpha|$). Furthermore, in the limit of very strong noise, a localized configuration turns out to be almost stable.

Since in both cases, $\bar{\mathbf{x}} \to 0$ exponentially, we have that

$$\bar{\rho} \to \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}, \tag{10}$$

which says that in any case we have almost complete decoherence at large times, the off-diagonal elements being damped, whereas the diagonal ones carry the probabilities.

From (10) we do not conclude that an individual system is in one of the two configuration positions. In fact, from the stochastic equation (6) one can derive the set of linear equations

$$\dot{\overline{z^2}} = 4\alpha\overline{zy},$$
$$\dot{\overline{y^2}} = -4\alpha\overline{zy} - 4\beta^2\overline{y^2} + 4\beta^2\overline{x^2},$$
$$\dot{\overline{yz}} = -2\beta^2\overline{zy} + 2\alpha\overline{y^2} - 2\alpha\overline{z^2}. \qquad (11)$$

Using the condition $\overline{x^2 + y^2 + z^2} = 1$, one can replace $\overline{x^2}$ with $1 - \overline{y^2} - \overline{z^2}$ in the second of the above equations. For any $\beta \neq 0$ one finds that the solution converges to the stationary solution $\overline{x^2} = \overline{y^2} = \overline{z^2} = \frac{1}{3}$, $\overline{zy} = 0$. This means that the typical state is not localized (localization for all states would imply $\overline{z^2} = 1$). The off-diagonal terms are therefore always present for the density matrix associated to a single realization of the noise, only the average cancels them. A new ingredient is thus necessary to produce localization.

4. Nonlinearity

The effect of the interaction with the environment can be taken into account also considering a nonlinear term in the differential equations that describe the evolution of the density matrix. This kind of nonlinearity may occur when the Hilbert space of a quantum mechanical system with many degrees of freedom is replaced by the Hilbert space of a single object with few degrees of freedom. We do not enter here into this problem and we simply assume that α depends on the state ($\alpha = \alpha(x, y, z)$). For the sake of simplicity assume, as usual, that this dependence reduces to a dependence on the modulus square of the wave function. In our language it means that α depends only on z.

Also assume that:

(a) $\alpha(z)$ is an even function of $z : \alpha(z) = \alpha(-z)$;
(b) $\alpha(z)$ is zero at the poles: $\alpha(+1) = \alpha(-1) = 0$, positive otherwise and sufficiently smooth around the poles.

In the absence of noise, Eq. (3) still holds, with the only difference that α depends on z. The requirement (b) implies that a localized state remains, in fact, localized. Nevertheless, the system is not able to spontaneously localize. Notice that the first component x of the vector $\mathbf{x}$ remains constant during the motion. This means that there is no decoherence, and furthermore, that the system can never reach one of the poles. Indeed, the motion remains periodic, since we are on a two-dimensional variety. The only exception is when the system is initially on the meridian $x = 0$, in which case it moves along this meridian towards one of the poles producing localization, but this ensemble of initial conditions has probability zero.

In conclusion, nonlinear differential equations, like the equation which models the interaction with the environment, are not able to induce localization. Nevertheless, this goal can be achieved if one takes into account the simultaneous presence of these two different mechanisms: noise and nonlinearity.

5. Localization induced by noise and nonlinearity

Let us consider again the Hamiltonian (4) with $\alpha = \alpha(z)$; the previous requirements on $\alpha(z)$ are also assumed. The differential equation (6) which remain formally unchanged (the only difference is that α is no longer constant, but it depends on z), have two fixed points corresponding to the poles. What we can show is that, independent of the initial conditions, one has $z(t) \to \pm 1$. This convergence is not due to the attractiveness of the poles but to the fact that the motion along the meridians becomes more and more slow approaching the poles. In other words, the system stays for long time intervals around them, the distribution of this time interval having sufficiently long tails to guarantee that at the end, the system will spend almost all its time around a pole (it will be almost surely in a pole).

We can sketch how to show that the system localizes for large times; a rigorous proof being beyond the scope of this paper. The requirements on $\alpha(z)$ imply that it can be approximated around the poles by

$$\alpha(z) = \alpha_0(1 - z^2) + \cdots . \qquad (12)$$

We now prove that the limiting (steady) distribution is concentrated on the poles. Using Eq. (6) with the constant α replaced by (12) and Ito calculus, we find the differential equation for the product $\theta(z-z_c)y$. Then, taking the average, we have

$$\frac{d}{dt}[\overline{\theta(z-z_c)y}] = -2\beta^2\overline{\theta(z-z_c)y} -2\overline{\alpha(z)\theta(z-z_c)z} +2\overline{\alpha(z)\delta(z-z_c)y^2}, \qquad (13)$$

where $0 \le z_c \le 1$, and $\theta(\cdot)$ is the step function.

We can safely assume that any initial distribution on the surface of the unitary sphere will evolve, after a transient time, towards a stable distribution. For this stable distribution, the above time derivative $(d/dt)\overline{\theta(z-z_c)y}$ vanishes.

Furthermore, from Eq. (6), it also follows that

$$\frac{d}{dt}[\overline{\theta(z-z_c)}] = 2\overline{\alpha(z)\delta(z-z_c)y}. \qquad (14)$$

The above equation implies for the steady distribution $\overline{\delta(z-z_c)y} = 0$, which, in turn, implies $\overline{\theta(z-z_c)y} = 0$.

This last equality, inserted in (13), gives for the stationary distribution

$$\overline{\alpha(z)\theta(z-z_c)z} = \alpha(z_c)\overline{\delta(z-z_c)y^2}, \qquad (15)$$

which leads to

$$\lim_{z_c\to 1}\frac{\overline{\alpha(z)\theta(z-z_c)z}}{\alpha(z_c)\overline{\delta(z-z_c)y^2}} = 1. \qquad (16)$$

It is intuitive, and it can be also easily shown (again from (6)) that the relative difference between $\overline{\delta(z-z_c)y^2}$ and $\overline{\delta(z-z_c)x^2}$ vanishes in the limit $z \to z_c$, in fact the random rotation around the z-axis becomes very fast compared with the rotation around the x-axis. Therefore, since $x^2+y^2+z^2=1$, we can replace $\overline{\delta(z-z_c)y^2}$ with $\overline{\delta(z-z_c)(1-z^2)/(2)}$ in Eq. (16), which we rewrite as

$$\lim_{z_c\to 1}\frac{\int_{z_c}^{1}(1-z^2)z\rho(z)dz}{((1-z_c^2)^2/2)\rho(z_c)} = 1, \qquad (17)$$

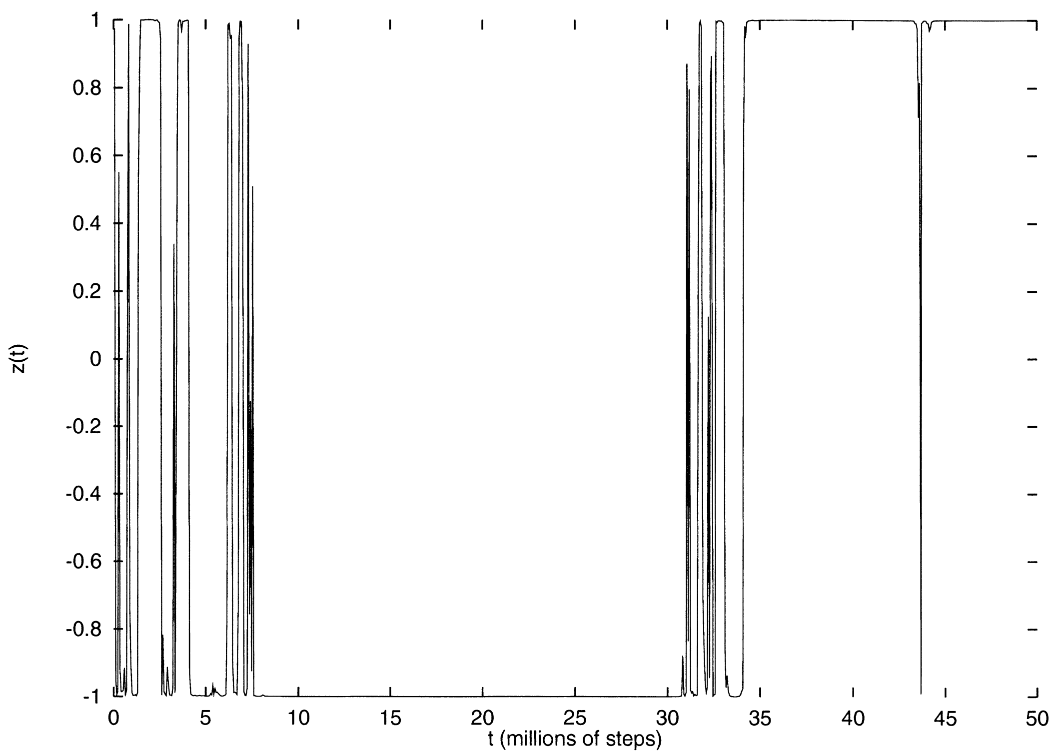

Fig. 1. A typical realization of $z(t)$ as function of t for $\alpha_0 = 1$ and $\beta = 7$. The differential equation (6) is numerically solved with a time step of 10^{-2}.

where we have used the expansion of $\alpha(z) \simeq \alpha_0 (1 - z^2)$ around the north pole and we have introduced explicitly the steady state probability $\rho(z)$ that the system is at a quote z.

Normalization implies that the probability distribution $\rho(z)$ cannot diverge around the north pole faster than $\rho(z) \simeq 1/(1 - z_c)^\gamma$ with $\gamma < 1$. With this assumption, we find that the above equation gives

$$\frac{1}{2-\gamma} = 1, \tag{18}$$

which cannot be satisfied for any normalizable distribution.

Finally, since (15) is satisfied for a distribution which is concentrated (Dirac's delta) in the north pole we find that this is the only possible stable distribution. Repeating the argument for $-1 \leq z_c \leq 0$, and taking into account the symmetry of the system (6) with respect to the changes $y \to -y$ and $z \to -z$, one can conclude that the steady distribution is made of two Dirac's delta distributions centered on the poles with equal weights.

Notice that this result implies again (10), i.e. $\bar{\rho}$ is equal one half of the identity operator for $t \to \infty$. Nevertheless, in this case, one has

$$\rho = \begin{cases} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} & \text{with probability } \frac{1}{2}, \\ \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} & \text{with probability } \frac{1}{2}, \end{cases} \tag{19}$$

and the density matrix decomposition corresponds to the combination of the two localized states.

Therefore, for what concerns decoherence nothing is changed, the important difference being that now $\overline{\rho^2} = \bar{\rho}$ for large times.

In Fig. 1, where $z(t)$ is plotted starting from a numerical solution of the differential equation (6) for $\alpha_0 = 1$ and $\beta = 7$, one sees clearly that the system

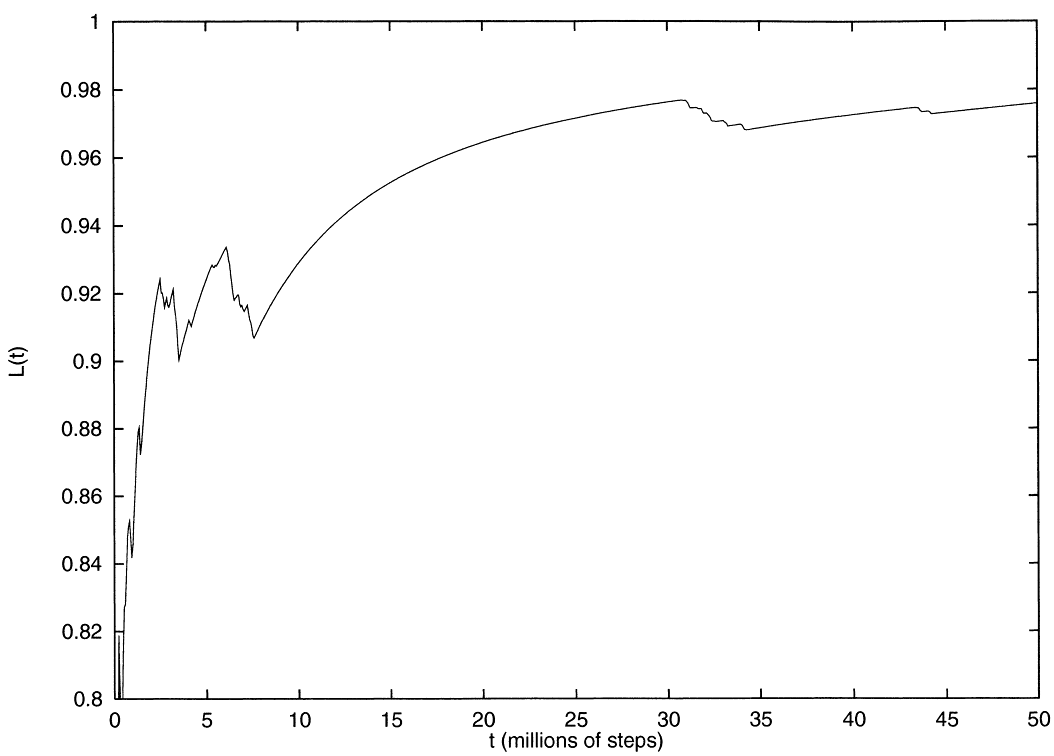

Fig. 2. $L(t)$ (19) as function of t for the same noise realization of Fig. 1 with $\alpha_0 = 1$ and $\beta = 7$.

spends a large part of the time in very narrow regions around the poles.

The time necessary to make a transition between the poles turns out to be negligible with respect to the long periods in which $z \simeq \pm 1$, which become infinitely large with t. Therefore, if one performs an observation of the system, it is almost sure to find it in a localized configuration. A useful quantity in order to show this fact is the time average of $z(t)^2$, defined by

$$L(t) = \frac{1}{t}\int_0^t [z(s)]^2\,\mathrm{d}s. \qquad (20)$$

This average tends to grow in time since the periods when $z(t)^2$ is substantially different from 1 become soon negligible, as shown by Fig. 2, where $L(t)$ is plotted for the same noise realization as Fig. 1.

6. Conclusions

We have presented a model where the coupling with the environment is represented both by a noisy potential and a nonlinear correction to the differential equations. This second effect should be a consequence of the interaction with the environment, whose degree of freedom, once integrated away, produces a feedback on the system. Nonlinearity and noise are not able to produce localization, while together they induce the system to spontaneously localize in one of its minimal energy configuration positions. Moreover, the localization site is chosen at random and it changes with time. In fact, the system can always make a transition between the two different macroscopic states, but the frequency vanishes for large time.

An interesting open question is if the same result can be reproduced also with an ohmic bath instead of the classical noise. In other terms, one wants to verify if localization occurs when the two configurations object interacts with an environment which is itself a quantum mechanical system with many degrees of freedom. This topic surely represents an interesting argument for future investigations.

The specific features of the model we have chosen are merely dictated by simplicity. Nevertheless, we would like to stress that we consider a genuine quantum dynamics without phenomenological dissipative terms in the Hamiltonian.

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