Real-space density-matrix renormalization-group study of the Kondo necklace

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A recently proposed density-matrix renormalization group is used to investigate the ground-state properties of the Kondo-necklace Hamiltonian. It represents a chain of XY interacting pseudospins that are Kondo coupled (J) to localized spins. The spin gap as well as the short- and long-range spin correlation functions are consistent with the existence of a smooth crossover at $J\approx 0.5$. For $J\leq 0.5$, the gap depends exponentially on $J^{-1/2}$ and the in-plane correlation function of the localized spins shows RKKY oscillations while the z one falls monotonically in contrast to the XY behavior. The correlation length diverges at $J=0$. For $J\geq 0.5$, the gap is linearly increasing with J, and the system is made of nearly independent singlets.

I. INTRODUCTION

Alloys of heavy-electron materials such as Ce, Yb, or U are found to exhibit a variety of low-temperature properties including antiferromagnetism, superconductivity, Kondo-insulator, and metal[1–3] At these low temperatures, the physical properties are nearly those of heavy-fermion liquids. The local moment and the conduction electron do not exist independently. Such a situation has also been observed recently in an organic chain compound where the localized spin degrees of freedom are strongly coupled to those of itinerant electrons.[4,5] The physical picture which describes these properties is that there is a competition between magnetic ordering and the Kondo effect. When valence fluctuation effects are neglected, the standard Hamiltonian for this problem is the Kondo lattice model (KLM), which is a generalization of the Kondo one-impurity problem. This Hamiltonian is written as

$$H_{\mathrm{KLM}}=-t\sum_{i\sigma}(c^{+}_{i+1\sigma}c_{i\sigma}+\mathrm{H.c.})+J\sum_{i}\mathbf{s}_{ic}\cdot\mathbf{s}_{\mathrm{if}}\ , \qquad (1)$$

where the conduction electron spin density on site i is $\mathbf{s}_{ic}$ and the f electron spin density is $\mathbf{s}_{\mathrm{if}}$.

The KLM has been widely studied in the last few years, especially at half filling. Monte Carlo calculations[6] as well as exact diagonalization,[7] real-space renormalization-group[8] approaches have led us to conclude that there is an unstable critical point at $J=0$ while the critical points $J=\pm\infty$, corresponding to the local antiferromagnetic and the ferromagnetic cases, respectively, are stable. Thus the ground state at $J=0$ is degenerate and a gap is opened for infinitely small values of J. Yu and White[9] have recently reached the same conclusion by means of a new version of the real-space renormalization-group technique. Their results also reveal that the spin gap is always smaller than the charge gap. Thus the low-energy properties of the KLM are driven by spin excitations rather than charge excitations. These conclusions are in qualitative agreement with the Doniach ansatz[10] which neglected the charge degree of freedom of the conduction electron. His Hamiltonian, called the Kondo-necklace model (KNM), cannot be directly related to the KLM but is expected to retain the fundamental competition between a magnetic state driven by the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction and a nonmagnetic state controlled by the Kondo mechanism. The KNM reads

$$H_{\mathrm{KNM}}=w\sum_{i}(t^{x}_{i}t^{x}_{i+1}+t^{y}_{i}t^{y}_{i+1})+J\sum_{i}\mathbf{t}_{i}\cdot\mathbf{s}_{i}\ . \qquad (2)$$

We set $w=1$ in the rest of the present study. A pseudospin chain $\mathbf{t}_i$ is here coupled to an ensemble of localized spins $\mathbf{s}_i$. These are all spin $\frac{1}{2}$. The rotational invariance of the KLM Hamiltonian is lost in the KNM. However, Doniach has calculated the weak-coupling limit and found that the scaling behavior of an individual spin $\mathbf{s}_i$ in the chain of pseudospins is equivalent to that of the one-impurity Kondo Hamiltonian.

We first review the results of previous calculations of the physical properties of the KNM. The first treatment of the KNM by Doniach[10] in the mean-field approximation led to the observation of a critical value of $J=J_c=1$. It described a transition from an antiferromagnetic state below J_c to a Kondo state above. The order parameter below J_c was observed to be proportional $\sqrt{1-J_c^2}$, a typical mean-field behavior. However, it is well known that the mean-field approach is not valid for such a system because of the important of quantum fluctuations at $T=0$ K. Jullien, Fields, and Doniach[11] went further by using a real-space renormalization-group method but obtained qualitatively similar conclusions. They calculated end to end correlation functions and found them to have finite value, even for an infinite lattice system. This indicated a long-range order in the small-J phase. They found $J_c=0.375$. However, this method leads to poor accuracy. For instance, the ground-state energy at $J=0$ agrees with the exact XY value only within 9–20 %. It is also known that the XY Hamiltonian does not exhibit any long-range ordering. Jullien *et al.*,[8] in a subsequent calculation, concluded the absence of a long-range order for all values of J, yet maintained their previous conclusion concerning the existence of a critical point at $J=0.375$.

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Scalettar *et al.*[12] carried out a Monte Carlo calculation of the KNM up to $N=16$ sites. They extrapolated the ground-state energy to the $N\rightarrow\infty$ limit with an estimated error of 0.5%. Their results contradict the real-space renormalization-group conclusions. The phase transition between the XY state and the Kondo state takes place at $J_c=0$. This study, however, is restricted to small lattice sizes. An accurate calculation for large lattices of such physical properties as the energy gap between the singlet and triplet states or the correlation functions is still necessary. We point out, concerning the singlet-triplet gap, that an attempt has been recently made by Santini and Sólyom to calculate it. They believe that a transition exists at $J_c=0.24$.[13] Finally, Strong and Millis[14] proposed a generalization of the KNM in which they introduced an anisotropic Heisenberg coupling within each of the two chains. The calculated the phase diagram of these two coupled chains system using a boson field approach. They found that a gap opens for nonzero values of the interchain Kondo coupling within a certain range of the intrachain couplings. This gap behaves as J^{α} where α is a function of the couplings. This phase diagram agreed qualitatively with the existence of a crossover, in the KNM, between a Kondo and an XY phase. Thus, the question is still open whether the KNM shows a ground-state phase transition or not.

In this paper, we apply a new version of real-space renormalization group to the KNM. This technique developed by White[15] differs fundamentally from the version used in previous studies. In the standard real-space renormalization-growth approach, one diagonalizes the Hamiltonian matrix between the states of two coupled blocks of spins and then keeps its lowest-energy states to define a new block of spins. This procedure has been shown to mistreat the boundary conditions which play an important role.[16] Indeed, although one couples two blocks at each iteration, this pair of blocks remains isolated from the rest of the chain. This is too constraining on the possible spin states of this superblock. White has shown that, in such cases, an accurate description of the system is given by the highest eigenvalues of the density matrix of the block instead of that of the Hamiltonian. The method of White, the density-matrix renormalization group (DMRG), has been successfully tested on Heisenberg chains and leads to extremely accurate results. For instance, the ground-state energy of both $s=\frac{1}{2}$ and $s=1$ chains has been obtained with up to nine-digit precision.

We have calculated the ground-state energy, the spin gap, and the short- and long-range correlation functions for lattices of up to a few hundred sites, keeping up to 80 states per block. We varied J from 0 to 5. We obtained typical truncation errors of 10^{-6} at $J=0.1$ and less than 10^{-10} at $J=5$. We also used the infinite system method with open boundary conditions. This approach, although less accurate than the finite system method,[15] allowed us to calculate satisfactorily the behavior of large systems. Our results elucidate the nature of the ground state of the KNM. The system is characterized by two regimes. For low values of J, medium-range RKKY oscillations are seen on the localized spins while the conduction spins will show XY oscillations. As the coupling increases, these oscillations decrease, eventually driving the system into a Kondo state in which the localized spin are drawn into singlet pairing with the conduction spins.

II. GROUND-STATE ENERGY

Let us first examine the ground-state energy per site versus J, for $0\leq J\leq 5$. For this calculation, we form the density matrix by projecting only the ground-state wave function.[15] We obtain the value -0.3183 at $J=0$. Comparing this value to the exact result of $-1/\pi=-0.318\,31$ allows us to estimate the quantitative error in our calculation. It is found to be less than 0.003%, better than the best extrapolation of the Monte Carlo calculations. For large J, the ground-state energy tends to $-\frac{3}{4}J$. For example, we have obtained the value -3.77 for $J=5$. This result is consistent with the strong-coupling expansion

$$E=-\frac{3}{4}J\left[1+\frac{1}{12}\left[\frac{1}{J}\right]^2+\cdots\right]. \tag{3}$$

One can note the high accuracy of the results. We will see later that despite this accuracy, the determination of the ground-state character is not straightforward.

III. SINGLET-TRIPLET GAP

The study of the gap is also important in order to understand the nature of the ground state. We show in Fig. 1(a) the value of the spin gap Δ versus J, for $0\leq J\leq 1$. The gap is defined here as the energy difference between the states having total spin S of 1 and 0. In the DMRG algorithm the states are labeled by the total z component of the spin S_z; the state with $S=1$ corresponds to the triply degenerate state having S_z equal to 0, 1, or -1. In order to improve the precision on the gap, we have built the density matrix projecting not only the ground state but also the first excited state. We have noticed that the truncation errors are in this case slightly larger. But this method has the advantage of leading to a better estimation of the gap because at each step, we keep the information on the first excited state. In the region $J>0.5$, the truncation errors are very small. We retrieve the results of previous calculations in this range: the gap is linear. But as J decreases, the accuracy also decreases and the gap gets smaller; thus the calculation in the interval $J<0.5$ becomes extremely delicate. To our knowledge, the only numerical study which has tried to clarify the gap behavior in this range of parameters is that of Santini and Sólyom.[13] These authors have studied clusters containing up to ten sites and have extrapolated their results to infinity. They came to the conclusion that the gap vanishes in a Kosterlitz-Thouless fashion at the critical value $J_c=0.24$. This was supported by the fact that at $J=0.325$, the gap is equal to 4×10^{-3}, at $J=0.3$, it is only 10^{-4}, and below $J=0.3$, it fluctuates between very small positive and negative values. We have not found such a behavior. Although our study is restricted to 100 sites, it is reasonable to think that if the tendency found by Santini and Sólyom exists, it should appear at this number of sites. But as we found, there is no large shift

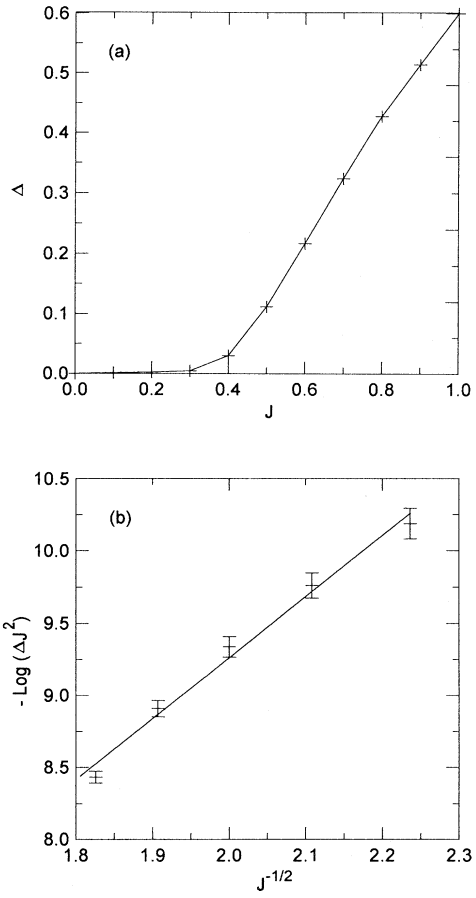

FIG. 1. (a) Spin gap Δ versus the coupling J. (b) $\mathrm{Log}(\Delta J^2)$ as a function of $1/\sqrt{J}$ for $J=0.2$, 0.225, 0.25, 0.275, and 0.3.

between $J=0.325$ and $J=0.3$ where the gap takes, respectively, the values 0.003 67 and 0.002 42. We note that the value 0.004 found by Santini and Sólyom at $J=0.325$ is consistent with ours. We arrived at the conclusion that for 100 sites, the gaps are close to that of the infinite system for those values of J of interest here. It is also interesting to study the mathematical behavior of the gap. We verified [see Fig. 1(b)] that it can be satisfactorily fitted by $J^{-2}\exp[-1/\sqrt{J}\,]$ as Ref. 12 suggested.

Tsunetsugu *et al.*[7] have recently calculated the spin gap of the half-filled KLM by means of exact diagonalization and infinite lattice extrapolation. The spin gap has two regimes. In the small coupling case, the spin gap behaves as $\Delta \propto \exp[-cst/J]$. A similar behavior is found in Ref. 6 where the Gutzwiller results for the symmetric Anderson lattice have been related to the Kondo lattice by means of the Schrieffer-Wolff transformation. In the strong-coupling case, the ground state is a set of on-site singlets. The lowest excited state is a triplet which can be obtained by breaking up one of the singlets. The energy cost in this process is J since the spin gap represents the energy of a singlet to triplet transition. The gap here behaves as $\Delta \propto J$. These results can be compared to ours. The change in the gap regime from exponential to linear behavior occurs near $J=0.5$. Since the KNM is expected to describe the spin excitations of the KLM, its gap may be expected to have similar behavior. So we conclude that in spite of the breaking of symmetry introduced in the KNM, both KLM and KNM belong to the same class of universality.

IV. CORRELATION FUNCTIONS

A. Short-range correlations

We have chosen to illustrate the short-range order by calculating correlation functions such as $G_s=\langle s_1^+ s_2^- \rangle$, $G_t=\langle t_1^+ t_2^- \rangle$, $G_{sz}=\langle s_1^z s_2^z \rangle$, $G_{tz}=\langle t_1^z t_2^z \rangle$, $G_s'=\langle s_1^+ s_3^- \rangle$, $G_t'=\langle t_1^+ t_3^- \rangle$, $G_{sz}'=\langle s_1^z s_3^z \rangle$, $G_{tz}'=\langle t_1^z t_3^z \rangle$, $G_{szi}=\langle s_0^z s_i^z \rangle$, and $G_{tzi}=\langle t_0^z t_i^z \rangle$. These are plotted in Figs. 2–4 as a function of J or of distance. The short-range gradually falls to zero above the value $J=0.5$, the value at which we have already seen the change of regime in the gap. It should be noted that the equal-distance correlation functions for spins and pseudospins become nearly equal around this value of the coupling. Finally, the localized-delocalized spin correlation function $G_{st}=\langle \mathbf{s}\cdot\mathbf{t} \rangle$ (not illustrated) rapidly decrease as J increases, approaching the value $-\frac{3}{4}$which is consistent with the fact that at strong J, the system condenses into independent singlets on each site. For instance, we obtain -0.25, -0.69, and -0.748 for J equal to 0.1, 1, and 5, respectively.

For $J<0.5$, the spin correlation functions are observed to be quite different from the pseudospin ones. The latter rapidly tend to the XY chain values as J decreases. The former ones, as borne out by Figs. 3 and 4, are typical of a RKKY chain. Indeed, we have simulated a small chain of spins interacting through the RKKY interaction generated by the pseudospins and found the behavior of G_{szi} to have the same characteristic monotonic decrease with distance as the $J=0.1$ curve of Fig. 4. This correlation function proves to bear the signature of RKKY intrachain correlations in the KNM for small J. Such a behavior can be understood by the fact that the effective

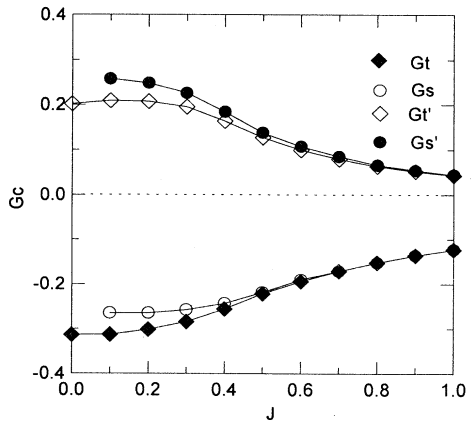

FIG. 2. In-plane nearest-neighbor and next-nearest-neighbor correlation functions, G_C, versus J, for the conduction spin chain ($C=t$ and t') and the localized spin chain ($C=s$ and s').

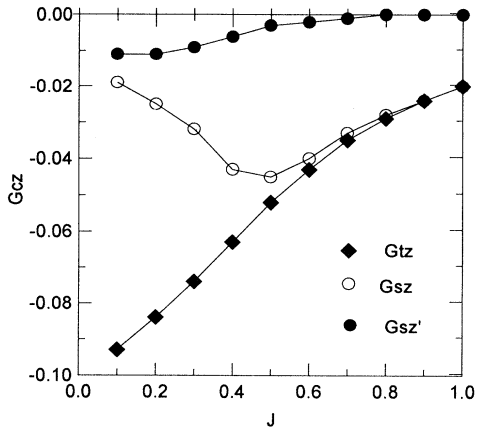

FIG. 3. The z component of the nearest-neighbor and next-nearest-neighbor correlation functions, G_{CZ}, versus J, for the conduction spin chain ($C=t$) and the localized spin chain ($C=s$ and s').

coupling between the localized spins is $J_{xy}\sim(-1)^{i-1}/(i)^{-1/2}$ in the plane, and $J_z=0$ if i is even and $J_z\sim 1/i^2$ if i is odd. This behavior should persist to distances of the order of the correlation length $\xi\propto\Delta^{-1}$.

B. Long-range correlations

Although we have obtained satisfactory results on calculating energies or short-range correlation functions at $J=0$, when $w=1$ between all the sites, we were unable to evaluate the asymptotic behavior of the correlation functions with equal accuracy. In order to avoid end effects, we first build our lattice up to 50 sites and then we start the calculation. We have calculated intersite correlations for distances up to 25 lattice sites. In the XY chain, the correlations functions decay as $i^{-1/2}$, i being the distance between the pseudospins, but we found local values of the exponent which are typically 0.52 at $i=10$ and 0.60 at $i=20$. This is not due to the precision of the method but rather to the effect of the open boundary conditions which induce a strong alternation of the bond strength near the ends on an $s=\frac{1}{2}$ system.[15] These alternations decay very slowly as the size increases. But they can be suppressed by the introduction of smooth boundary conditions.[17] In our case, we artificially set $w=0.18$ between sites at the end of the chain, and we obtained a very good agreement with the exact result. The calculated values of the correlation functions reproduce the exact one (see Table I) at up to 7×10^{-4}. We have noticed that these oscillations become negligible at nonzero values of J, even at $J=0.01$, so that the trick used above is not necessary in the case $J>0$. We plot in Fig. 5 the results for the in-plane correlation functions $G_{si}=\langle s_0^+ s_i^-\rangle$ where the s_0 spin is taken in the middle of the chain. It presents RKKY antiferromagnetic oscillations which slowly vanish as the distance increases. But, as already observed in Fig. 4, there are no oscillations for small J in the z direction and the decay with distance is more rapid.

TABLE I. The first six calculated values of the transverse correlation functions in an XY chain of length 100 versus the exact values. The values of the exact result are taken from Ref. 18.

i	G_{tiexa}	G_{ticalc}
1	0.3184	0.3177
2	0.2026	0.2027
3	0.1720	0.1715
4	0.1460	0.1461
5	0.1322	0.1318
6	0.1194	0.1197

It is interesting to look at the decay of the correlations as a function of the distance. In the Monte Carlo calculations,[12] the authors found that the exponent of a power-law decay increased from the value 0.5 at $J=0$. This would have precluded any possibility of a ground-state Kosterlitz-Thouless transition as proposed in Ref. 13

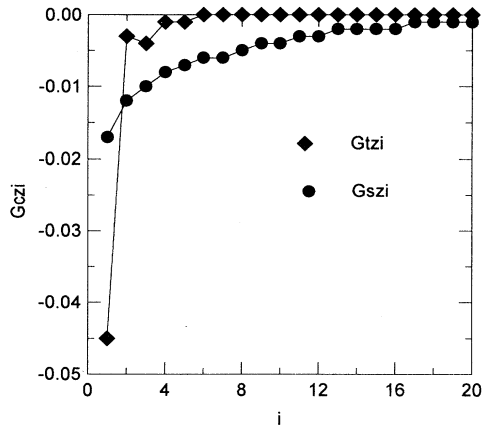

FIG. 4. The z-component correlation function, G_{CZi}, of the conduction spin chain ($C=t$) and the localized spin chain ($C=s$), as a function of the interspin distance i for $J=0.1$.

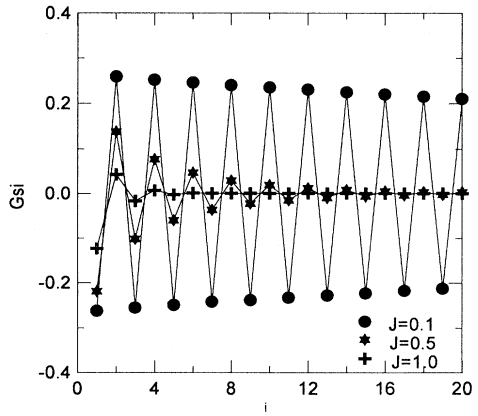

FIG. 5. In-plane correlation function G_{Si} between two localized spins as a function of the distance. One of the spins is taken in the middle of the chain.

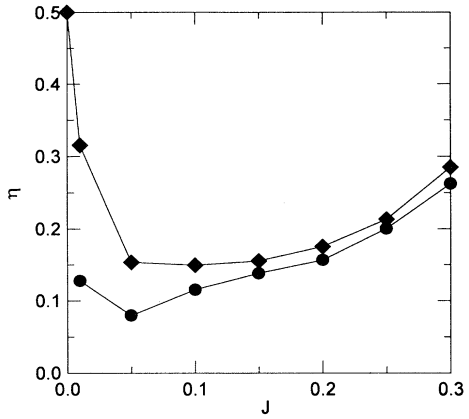

FIG. 6. The calculated exponent η for the conduction spin chain (diamonds) and the localized spin chain (circles), for an algebraic decay versus J of the in-plane correlation function.

since the power-law exponent must equal 0.25 at the transition. We have obtained the in-plane exponents from our 25-site correlation function calculations. Figure 6 shows that our results disagree with those of the Monte Carlo calculations. Starting from $J=0$, the exponent decays until $J=0.1$ for both the conduction and localized spin chains. It then increases. Note that it takes the value 0.25 at a coupling value of roughly $J=0.27$. The reason for the discrepancy surely has to do with the much larger chain lengths we were able to use. 25 Sites is still, however, shorter than the correlation length $\xi \propto \Delta^{-1}$ for $J<0.3$. We have thus calculated the RKKY quantum regime exponents and cannot observe the asymptotic exponential behavior caused by the opening of the small gap. Interestingly enough, we obtain a "critical" coupling value close to $J_c=0.24$ of Ref. 13. This may well point to a natural tendency for a Kosterlitz-Thouless-type instability of the quantum regime, thwarted by the Kondo mechanism.

V. CONCLUSION

The DMRG method has allowed us to investigate the properties of the KNM. This method shows better accuracy than the Monte Carlo calculations or the standard real-space renormalization group (RG). The study of the KNM shows three interesting values of the coupling: $+\infty$, 0.5, and 0. The point $+\infty$ is a stable fixed point where the system consists of on-site independent singlets. The point $J=0$ is the XY limit where the system shows algebraic magnetic order. The question was to know if there is a phase transition at a finite value of the coupling. In their previous RG calculations, Jullien *et al.* have concluded the existence of a phase transition at $J=0.5$ because they found no gap below this value. But then the examination of the correlation functions by Scalettar, Scalapino, and Sugar[12] by means of the Monte Carlo method indicates an absence of a critical behavior at finite J. Our results indicate that the ground state is a singlet for all nonzero values of J. This shows that the system does not present a phase transition at finite J. Thus our results agree with the Monte Carlo conclusion that the transition occurs at $J=0$. But we emphasize the fact that the Monte Carlo conclusions were based on system sizes which were too small to capture certain behaviors in the thermodynamic limit. The point $J=0.5$ can be seen as the onset of a smooth crossover from the small-J RKKY medium-range correlation regime to the Kondo regime. Indeed, the small-J regime in which RKKY oscillations dominate is not a real antiferromagnetic state with a long-range order (LRO). It is well known that in a one-dimensional system, the transverse fluctuations tend to reduce a LRO to a quasi-LRO which still have a collective mode and a correlation function that shows algebraic decay. Furthermore, in the case of the KNM, our results display the fact that this quasi-LRO is inhibited by the presence of a small gap which is probably a reminiscence of the singlet-triplet splitting found at higher values of J. Finally, we noted the analogy between the Kondo necklace and the Kondo lattice models.

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