Cluster Development in an N-Body Problem*

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The procedure for generating useful cluster development in problems dealing with the Jastrow wavefunction, as proposed by Wu and Feenberg, is discussed in detail. The existence of the expansion is proved to all orders; also a simple rule is given for computing the expansion coefficients. The result can be considered as a generalization of the Ursell–Mayer formulas.

I. INTRODUCTION

In the statistical and quantum mechanical treatment of an N-body system, one often needs the technique of the Ursell–Mayer-type cluster expansion in evaluating physical quantities of interest. In the general case the quantity considered may be a function of N distinct indices. For example, in case of fermions, when a trial wavefunction involving N single-particle orbitals is used to describe the system, all quantities calculated for this system depend on the N orbitals explicitly. This kind of problem was first taken up by Jastrow who introduced a correlated wavefunction containing a factor describing the correlation among particles in addition to a Slater determinant composed of plane-wave orbitals. The mathematics of the cluster expansion in problems involving such wavefunction has been discussed exhaustively by Hartogh and Tolhoek in a series of papers in which general expansion theorems are fully developed. On the other hand, a much simpler formalism which is more general, in the sense that the problem of Jastrow wavefunction appears as a special case of its application, was introduced by Iwamoto and Yamada. Considering the complicated notation and the large quantity of combinatorial algebra involved in the discussion of Hartogh and Tolhoek, an alternative rigorous treatment along the more general lines indicated by Iwamoto and Yamada seems desirable. However it is rather difficult to demonstrate the general character of the cluster expansion by the method of Iwamoto and Yamada; also the existence of the expansion for arbitrary order is not easily proved. An alternative procedure which retains the essential simplicity and directness of the Iwamoto–Yamada approach has been found by Wu and Feenberg and used by them to compute numerical results in a study of the fermion liquid. It is therefore the purpose of this note to present a further detailed discussion of the latter procedure. The existence of the expansion is proved to all orders; also a simple rule is given for computing the expansion coefficients. The result reduces to the Ursell–Mayer formulas if one neglects the difference between all indices and, therefore, our formula is, in a sense, a generalization of the Ursell–Mayer formalism.

II. PROCEDURE OF CLUSTER DEVELOPMENT

As is well-known, the cluster-expansion procedure is usually used in evaluating the logarithm of quantity which behaves like exponential function of N. In applications, the quantity of the order of $e^{aN}$ often has an integral form

$$K_{12...N} = \int W_{12...N}(\tau_1, \tau_2, \ldots, \tau_N) \, d\tau_1 \, d\tau_2 \cdots d\tau_N,$$

(1)

in which the indices 1, 2, ..., N refer to, e.g., the N different single-particle orbitals involved in the trial wavefunction. The function $W$ is symmetric in all coordinates $\tau_1, \tau_2, \ldots, \tau_N$ of the N particles and the subscripts 1, 2, ..., N. A systematic way to handle the problem, i.e., to evaluate in $K_{12...N}$ is as follows. First one defines the reduced $K$ quantities by specifying certain rules by which one generates the $K$ quantities of one index, two indices, etc. For example if $K_{12...N}$ is given by Eq. (1), one way to define the reduced $K$'s is

$$K_1 = \int W_1(\tau_1) \, d\tau_1,$$

(2)

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\[ K_{mn} = \int W_{mn}(\tau_1, \tau_2) \, d\tau_1 \, d\tau_2, \text{ etc.}, \quad (3) \]

with \( l, m, n \ldots \) referring to different indices in the set \( 1, 2, \ldots, N \). The range of integration is the same in all these integrals. Then the following relations generate a set of \( X \) quantities, or a set of cluster integrals:

\[ K_i = X_i, \]
\[ K_{im} = X_i X_m + X_i X_{im}, \]
\[ K_{imm} = X_i X_m X_n + X_i X_{imn} + X_m X_{in} + X_m X_{im} + X_{imm}, \cdots, \]

until finally one reaches

\[ K_{12 \ldots N} = \sum_{\substack{m_1 \text{ factors} \in N \setminus \{i\} \ldots \{N\} \setminus \{i\} \cdots \{N\} \setminus \{i\}}} \left\{ \cdots X_i \cdots X_i \right\}, \]
\[ \times \left\{ \cdots X_{im} \cdots X_{im} \right\}, \cdots, \]

in which the summation extends over all possible products subject to conditions (i) no repeated indices; (ii) permutation within a bracket not distinguishable. Each \( K \), hence \( X \), is symmetric with respect to its indices.

As stated earlier, in application we are interested only in the cases

\[ \ln K_{12 \ldots N} \sim O(N). \]

In fact if the rule that specifies the reduced \( X \)'s is taken properly, one always has

\[ X_{(m \text{ ind} \text{ cases})} \sim O(N^{1-m}), \]

and Eq. (6) follows as a result of Eq. (7), as we shall see. Both Eqs. (6) and (7) are checked easily in the special case of Mayer's cluster expansion for a classical imperfect gas for which all \( X \)'s having the same number of indices are identical.

It is convenient to write

\[ K_{12 \ldots N} = X_1 X_2 \ldots X_N I, \]
\[ x_{1m \ldots n} = X_{1m \ldots n} / X_1 X_m \ldots X_n, \]
\[ I = 1 + \sum_{m < n} x_{mn} + \sum_{l < m < n} x_{lmn} \]
\[ + \sum_{k < l < m < n} (x_{kl} x_{mn} + x_{km} x_{ln} + x_{km} x_{ln} + x_{km} x_{ln}) \]
\[ + \cdots; \]

then

\[ \ln K_{12 \ldots N} = \sum_{i=1}^{N} \ln X_i + \ln I. \]

The problem is now reduced to the evaluation of \( \ln I \). At this stage, Iwamoto and Yamada\(^8\) write down a set of differential equations and solve the problem by constructing successive approximate solutions. The extension of their method to arbitrary order is difficult to carry out. In particular, the differential equations must be written down with great care in order to not overcount many terms. In the following, we shall first outline the alternative procedures suggested by Wu and Frengend\(^7\) and then extend the discussion to all orders.

Let \( I_{m \ldots n} \) denote the function generated by omitting all terms in Eq. (10) containing indices in the set \( l, m, \ldots, n \). Then it is easy to see that in Eq. (10) the coefficient of the factor \( x_{mn} \) is exactly \( I_{m\ldots n} \) of \( x_{mn} \) is \( I_{m\ldots n} \) etc. It follows that Eq. (10) can be rewritten as

\[ I = I_q + \sum_m x_{qm} I_{qmn} + \sum_{m < n} x_{qmn} I_{qmn} \cdots \]
\[ + \sum_{m < n < \cdots < l} x_{qmn \ldots l} I_{qmn \ldots l} \cdots + x_{12 \ldots N}. \quad (12) \]

Now we write

\[ \ln I = G, \]
\[ \ln I_q = G_q = G - H_q, \]
\[ \ln I_{qm} = G_{qm} = (G - H_q - H_m)[1 + O(1/N)], \]

where \( G_{m \ldots n} \) denotes the function generated by omitting all terms in \( G \) containing indices in the set \( l, m, \ldots, n \). Retaining only the leading terms in the exponentials, we transform Eq. (12) into

\[ e^{H_q} = 1 + \sum_m x_{qm} e^{-H_m} \]
\[ + \frac{1}{2!} \sum_{mn} x_{qmn} e^{-\left(H_m + H_n\right)} + \cdots. \quad (14) \]

Here the convention that any \( x \) with repeated indices vanishes, i.e. \( x_{x \ldots x} = 0 \), is introduced. We emphasize that the substitutions Eq. (13) will be justified by actually determining \( G \).

Both sides of Eq. (14) and also each multiple sum are now independent of \( N \) so that a formal expansion of the exponentials is permissible. Taking the logarithms of the left- and right-hand members of Eq. (14), one obtains

\[ H_q = W - \frac{1}{2} W^2 + \frac{1}{3} W^3 - \cdots, \quad (15a) \]
\[ W = \sum_x x_{xm} \left[ 1 - H_m + \frac{1}{2!} H_m^2 - \cdots \right] + \frac{1}{2!} \sum_{mn} x_{qmn} \]
\[ \times \left[ 1 - (H_m + H_n) + \frac{1}{2!} (H_m + H_n)^2 - \cdots \right] + \cdots. \quad (15b) \]

As the equation stands, \( H_q \) can be generated by an\(^8\) We are indebted to Dr. Iwamoto for this remark.

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obvious iteration procedure. Indeed, we get for the first few terms

\[ H_{e} = \sum_{m} x_{mn} \]

\[ + \sum_{mn} \left( \frac{1}{2} x_{mn} - \frac{1}{2} x_{mxn} \right) + \cdots, \]  

(16)

which, in turn, produces

\[ G = \frac{1}{2!} \sum_{m} x_{mn} + \sum_{imn} \left( \frac{1}{3!} x_{iimn} - \frac{1}{2} x_{iimxn} \right) + \cdots, \]

(17)

as observed from the relation

\[ H_{e} = G - G_{e}. \]  

(18)

This observation is best demonstrated if one starts from the expression of \( G \) given by Eq. (17) and uses Eq. (18) to compute \( H_{e} \); then

\[ H_{e} = \frac{1}{2!} \sum_{m} x_{mn} + \sum_{imn} \left( \frac{1}{3!} x_{iimn} - \frac{1}{2} x_{iimxn} \right) + \cdots \]

\[ - \left[ \frac{1}{2!} x_{mn} + \sum_{mcm} \left( \frac{1}{3!} x_{nmcm} \right) \right] = \frac{1}{2} \sum_{m} \left( x_{mn} + x_{mcm} \right) \]

\[ + \sum_{mn} \left[ \frac{1}{3!} \left( x_{mcm} + x_{mcm} + x_{mcm} \right) \right] - \frac{1}{2} \left( x_{mcm} + x_{mcm} + x_{mcm} \right) \]

(16')

which is identically Eq. (16) on taking account of the symmetry of the \( x \)'s in the indices. Clearly the ratio between the coefficients of \( \sum_{mn} x_{mn} x_{mn} \) and \( \sum_{mn} x_{mn} x_{mn} \) in Eq. (16) must be 1 : 2 in order to generate the term \( \sum_{imn} x_{im} x_{mn} \) in \( G \). The necessity of such correlation between the coefficients in the expansion of \( H_{e} \) persists to all orders. The explicit statement of such correlation will be made after we introduce the diagrammatical representation below. Also one easily checks, with the help of Eqs. (7) and (9), that the first three terms of Eq. (17) are of the order \( O(N) \). This linear dependence on \( N \) also persists to all terms of \( G \). This fact follows from the structure of Eq. (15b) which tells us that the inclusion of each \( m \) index \( x \sim O(N^{1-m}) \) brings in exactly \( m - 1 \) free summations, and hence a factor \( N^{1-m}N^{m-1} \sim O(1) \).

A diagrammatical representation which will facilitate our discussion is now introduced. In the following, the \( x \)'s are called elements. An \( m \)-index element is imagined as a rigid frame with \( m \) holes (or vertices) attached to it: open holes represent the dummy indices of a summation, and a black or solid hole (indexed by \( q \)) is not summed over. No meaning is attached to the order of holes in an element (symmetry of an element in all indices). A collection of elements (i.e., a product of \( x \)'s) is called a diagram. The meaning of some simple diagrams are given by Fig. 1. A diagram is singly connected if all elements of the diagram are connected without forming any closed path; i.e., each hole common to two or more elements is an articulation which, if omitted, would dissociate the diagram into disconnected parts or branches. The degeneracy \( S \) of a hole with respect to a diagram is the number of holes equivalent to it because of the symmetry of the elements in the indices. In counting the degeneracy, we make no distinction between the black and white holes. Thus \( S = 2, 1 \) for the black holes of the diagrams of Figs. 1(a) and 1(b), respectively. Also \( S = m \) for the holes of a single \( m \)-vertex element. It is also convenient to define the symmetry number \( T \) of a diagram as the number of ways one can permute a definite set of distinct numbers attached to the open holes of the diagram without changing the topology of the diagram. For example, \( T = 1, 2, 2 \) for the diagrams of Figs. 1(a), 1(b), 1(c), respectively. Also \( T = m! \) for a single \( m \)-vertex element with no black hole, and \( T = (m - 1)! \) for the same element when one of the holes is black. It is clear that if in a diagram a black hole is replaced by an open hole, the symmetry number is changed from \( T \) to \( S \) where \( S \) is the degeneracy of the hole under consideration.

With this diagrammatical notation, it is readily observed from the structure of Eq. (15) that each term in the expression of \( H_{e} \) can be represented by a singly connected diagram with one black hole. In fact one can always find terms in Eq. (16) corresponding to an arbitrary diagram. Therefore we write

\[ H_{e} = \sum_{m} h_{e} \left( \text{all distinct singly connected diagrams with one black hole} \right), \]

(19)

with appropriate coefficient \( h_{e} \) for each diagram. The correlation among the coefficients \( h_{e} \) to ensure the existence of \( G \) is now clear: consider two diagrams
composed of the same collection of elements which differ only by the different positions taken by the black holes [e.g., Figs. 1(a) and 1(b)], the criterion is simply to require the ratio of their \( h \) coefficients be [see Eqs. (16) and (16')] 

\[
h_a/h_b = S_a/S_b = T_b/T_a,
\]

with \( S_a, T_a; S_b, T_b \) referring to, respectively, the corresponding degeneracies of the black holes and the symmetry numbers. In the last step of Eq. (20) we have used the relation

\[
S_a T_b = \begin{cases} \text{the symmetry number of the diagram if} & \\
\text{(the black hole is replaced by an open hole)} & 
\end{cases}
S_b T_a.
\]

Once Eq. (20) is established, one has immediately

\[
G = g \left( \text{all distinct singly connected diagrams with no black holes} \right),
\]

in which the coefficient \( g \) of an arbitrary diagram is given by the following procedure. First one changes (any) one of the holes in this diagram into a black one and looks for the coefficient \( h_a \) of this new diagram in Eq. (19). If the degeneracy of the black hole is denoted by \( S_a \), then

\[
g = h_a/S_a.
\]

Therefore our problem is to show the validity of Eq. (20) and to obtain an explicit expression for \( h_a \). To this end we state the following Lemmas to be proved in the Appendix.

**Lemma A.** In the expansion of \( H_a \), let \( h_1, h_2, \ldots \) denote the coefficients of diagrams in which the black hole is not an articulation, and \( h_a \) the coefficient of a black hole in which the black hole is an articulation having \( n_1, n_2, \ldots \) identical branches with coefficients \( h_1, h_2, \ldots \), respectively. Then

\[
h_a = (-1)^{n-1}(n - 1)! \prod_i h_i^{n_i}/n_i!,
\]

where \( n = \sum_i n_i \) is the total number of branches at the articulation.

**Lemma B.** The coefficient \( h_a \) of an arbitrary diagram in Eq. (19) is given by

\[
h_a = \frac{1}{T_a} \prod \left( \text{all holes of} \right) \left( -1 \right)^{n_i-1}(n_i - 1)!,
\]

in which \( T_a \) is the symmetry number of this diagram and \( n_i \) the number of elements connected by the \( i \)th hole \((n_i = 1 \text{ if the hole is not an articulation}).

An immediate consequence of Lemma B is Eq. (20). Therefore we have completed the proof that the expansion of \( G \) exists. Finally upon combining

\[
G = \frac{1}{n} \left( \text{fig.} \right)\left( \text{fig.} \right)\left( \text{fig.} \right)\left( \text{fig.} \right) + \frac{1}{2} \left( \text{fig.} \right) - \frac{1}{2} \left( \text{fig.} \right) + \frac{1}{2} \left( \text{fig.} \right) + \cdots
\]

**Fig. 2.** Diagrammatical equation for \( G \) up to terms involving six indices.

Eqs. (23), (25), and (21), the coefficient \( g \) belonging to an arbitrary diagram in Eq. (22) has the explicit form

\[
g = \left( \frac{1}{\text{symmetry number of the diagram}} \right) \times \prod \left( -1 \right)^{n_i-1}(n_i - 1)!. \tag{26}
\]

This concludes the derivation of the expansion formula for \( G = \ln I \). We give in Fig. 2 the explicit expression for \( G \) up to terms involving six indices. As checked easily, this result reduces to the Ursell-Mayer expansion if the cluster integrals involving the same number of indices are all identical.

**III. CONCLUSION**

We have shown that the logarithm of the quantity \( I \) of Eq. (10) can be expanded into a sum of terms represented by singly connected diagrams in the form of Eq. (22), with Eq. (26) furnishing an easy way to determine the expansion coefficients. We must note that terms down by a factor \( 1/N \) are neglected in the result. Also, the expansion is useful only when it converges fast enough so that the leading terms produce a good approximation. This seems, indeed, to be the cases in application.\(^4\)\(^7\)

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APPENDIX

Proof of Lemma A: The diagram with the black hole having \( n \) branches clearly comes from the term \((-W)^n/n\) of Eq. (15a). The multiplicity for occurrence of such a diagram in the expansion of \( W^n \) is \( n!/\prod n_i! \), with coefficient \( \prod h_i^n \). Upon combining these with the factor \((-\gamma)^n/n\), Eq. (24) is derived.

Q.E.D.

Proof of Lemma B: Lemma B will be proved by induction. First, it is obvious from Eq. (15) that Lemma B holds for a single \( m \)-vertex element for which

\[
h_a = 1/(m - 1)! = 1/T_a.
\]

Therefore it remains only to show that Lemma B holds for any diagram if it applies to arbitrary diagram composed of fewer elements.

First let us consider diagrams having articulation black holes. Let the branches of the diagram be specified by the set \( \{n_1, h_1\} \) as stated in Lemma A; then the symmetry number of the diagram is given by

\[
T_a = \prod_i T_i^{n_i} n_i!,
\]

where \( T_i \) denote the symmetry numbers of the branches. Now, by assumption, Lemma B applies to diagrams composed of fewer elements so that the coefficient \( h_i \) of each branch is given by

\[h_i = \frac{1}{T_i} \prod \text{all holes of the branch} (-1)^{r_i-1}(n_i - 1)!. \]

The substitution of Eqs. (29) and (28) into Eq. (24) now yields

\[h_a = \frac{1}{T_a} \prod \text{all holes of the diagram} (-1)^{r_i-1}(n_i - 1)!. \]

Q.E.D.

Next consider the diagram in which the black hole is not an articulation. In the most general case, the black hole sits on an \( m \)-hole element, with \( p \) of the \( m \) holes attaching branches. In order to illustrate the essential points of the proof, we shall consider the case of \( p = 1 \) only. The proof for the general case can be constructed in a completely similar fashion.

Consider the diagram shown schematically in Fig. 3 in which the black hole sits on an \( m \)-hole element with one open hole attaching \( n \) branches denoted again by the set \( \{n_1, h_1, T_i\} \). The symmetry number of the diagram is now given by

\[T_a = (m - 2)! \prod_i T_i^{n_i} n_i!, \]

with the symmetry numbers \( T_i \) of the individual branches related to \( h_i \) through Eq. (29). The coefficient \( h_a \) of this diagram comes from the term \( W \) of Eq. (15a). More specifically it comes from the following terms:

\[
\frac{1}{(m - 1)!} \sum_{j_2 \cdots j_{m-1}} x_{j_2 \cdots j_{m-1}} \sum_{i=1}^{n_i} \sum_{k=1}^{n_i} \frac{(-H_i)_k}{k!}.
\]

Comparison of Eq. (31) with Fig. 3 indicates that we need to collect terms represented by the set of branches \( \{n_1, h_1, T_i\} \) in the expansion of \( H_i^k \). The first term \( H_1 \) contains only one such term. The second term \( H_i^1 \) contains more than one contribution. In fact, for each distinct way that the \( n \) branches are divided into two groups, there corresponds a contribution with one factor of \( H_1 \) contributing to one group of branches, and another \( H_1 \) to the other group. The multiplicity for occurrence of such terms in the expansion of \( H_i^k \) is 1 if the two groups are identical, and 2 otherwise. In general for the term \( H_i^k \) we consider all the distinct ways that the \( n \) branches are divided into \( k \) groups of which \( \beta_1, \beta_2, \ldots, \beta_k \) are identical. Let the \( h \) coefficients of these groups be denoted by \( \bar{h}_1, \bar{h}_2, \ldots, \bar{h}_k \), respectively. Then for each distinct way that the
\( n \) branches are divided, there corresponds, in the expansion of \( H^*_k \), a contribution to the coefficient \( h^*_a \) with multiplicity \( k! / \beta_1 ! \beta_2 ! \cdots \beta_n ! \). It follows then from Eq. (31)

\[
h^*_a = \frac{1}{(m - 2)!} \sum_{k=1}^{n} \frac{(-1)^k}{k!} \times \prod_{\beta_1, \beta_2, \cdots, \beta_n} \frac{k!}{\beta_1 ! \beta_2 ! \cdots \beta_n !} h^*_k, \tag{32}
\]

in which \( (\beta_1 \beta_2 \cdots \beta_n) \) denotes the summation taken under the restriction \( \beta_1 + \beta_2 + \cdots + \beta_n = k \). Now the coefficients \( \tilde{h}_1, \tilde{h}_2, \cdots, \tilde{h}_n \) can be obtained by Lemma A. However it proves useful at this point to note that the factor \( (n - 1)! / \prod n_i ! \) appearing in Eq. (24) is just the number of distinct ways to perform cyclic permutations on the group of \( n \) branches (among which \( n_1, n_2, \cdots \) are identical). Using this interpretation of Lemma A for the expressions of \( \tilde{h}_1, \tilde{h}_2, \cdots, \tilde{h}_n \), we get

\[
\tilde{h}_1^1 \tilde{h}_2^2 \cdots \tilde{h}_n^n = (1)^{n-k} \prod_{i} h^*_i. \tag{33}
\]

Substituting Eq. (33) into Eq. (32), we have

\[
h^*_a = \frac{1}{(m - 2)!} (-1)^n M \prod_{i} h^*_i, \tag{34}
\]

where

\[
M = \sum_{k=1}^{n} \frac{1}{\beta_1 ! \beta_2 ! \cdots \beta_n !} \prod_{\text{product of the number of distinct cyclic permutations of the branches in each group}}
\]

\[
= \sum_{k=1}^{n} \frac{1}{\beta_1 ! \beta_2 ! \cdots \beta_n !} \prod_{\text{the number of distinct ways one can permute the \( n \) branches under the particular grouping by performing cyclic permutations within each group while the groups are unnumbered}}
\]

\[
= \sum_{k=1}^{n} \frac{1}{\beta_1 ! \beta_2 ! \cdots \beta_n !} \prod_{\text{the number of distinct ways one can permute the \( n \) branches by first dividing into unnumbered groups and then performing cyclic permutations within each group}}.
\]

It is well-known that each permutation of a collection of objects can be analyzed into groups of cyclic permutations in an unique way. Therefore also

\[
M = \frac{n!}{\prod n_i !}. \tag{35}
\]

The substitution of Eqs. (29) and (35) into Eq. (34) and the introduction of Eq. (30) now yields Eq. (25).

Q.E.D.

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**Strict Localization**

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A complete characterization for a general quantum field theory is given of the strictly localized states introduced by J. Knight. It is shown that each such state can be generated from the vacuum by a partially isometric operator. Necessary and sufficient conditions are given for the superposition of such states to be also strictly localized. Finally, it is shown that there is a connection between the von Neumann type of the ring generated by the field operator in a finite region and the possibility of constructing strictly localized states.

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**I. INTRODUCTION**

The notion of strictly localized states has recently been introduced by Knight.\(^1\) Let \( \varphi(x) \) be a complete, local, scalar Hermitian field. Let \( \Omega \) denote the vacuum state. Then a state \( \Psi \) is said to be strictly localized in a region \( G \) of Minkowski space if for any \( n \),

\[
\langle \Psi, \varphi(x_1) \cdots \varphi(x_n) \Psi \rangle = \langle \Omega, \varphi(x_1) \cdots \varphi(x_n) \Omega \rangle,
\]

when all the \( x_1 \cdots x_n \) are outside \( G \).

Knight has shown, for the case of the free field, that such states cannot contain a finite number of particles. He has also shown that states of the form

\[
e^i A \Omega,
\]

where \( A \) is a smooth polynomial in the field in a

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