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The infinite-range hopping approximation for a binary alloy. Exact Eigenstates

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ABSTRACT. We find exact eigenstates for the infinite-range hopping approximation to binary alloy disorder. We show how the determinants can be rearranged to get the exact solution. The eigenstates are well defined and not smeared as in CPA. To get the thermodynamic limit we find it necessary to scale the hopping term t by dividing by z (the number of neighbors) and not by $\sqrt{z}$ as adopted for the infinite dimension model by other authors.

RESUMEN. Encontramos autoestados exactos para la aproximación de rango infinito de la aleación binaria. Mostramos también cómo hay que reorganizar los determinantes para obtener la solución. Los autoestados están definidos por deltas en contraste con la CPA que da bandas. Para obtener el límite termodinámico vemos que el escaleo del término de salto t debe ser z (el número de vecinos) y no su raíz cuadrada como sucede en la aproximación de dimensión infinita de otros autores.

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1. INTRODUCTION

It is of current interest in solid state physics to study the tight-binding model which in the most difficult limits has two ingredients: correlation interaction and disorder. The first of these leads to states with different occupation number, whereas the second involves states that are no longer translationally invariant. Here we will present a solution with the disorder ingredient only, leaving the correlation interaction for further studies. Recently there has been increased interest in the so-called infinite dimension of the hopping term of the tight-binding part. It was first introduced by us [1] with the following scaling: $t' = t/z$, where t is the tight-binding hopping term and z is the number of nearest connected neighbors. It was called the infinite-range hopping model. The scaling is necessary to have the energy as a finite quantity. After that Volhardt *et al.*, [2] have published a series of papers where, using the same idea they scale: $t' = t/\sqrt{z}$ arguing that it is essential to obtain a proper density of states.

The completely connected t-model has its origin in the Sherrington-Kirkpatrick model for a classical spin-glass [3] where much work has been achieved. Our scaling of t [1] is the same as appears in the spin model [3]. The picture we have in mind is that of a big cluster with all the sites connected by a hopping t of equal strength. This somewhat

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$$\begin{array}{cccccc}
\epsilon & -t & -t & -t & -t & -t \\
-t & \epsilon & -t & -t & -t & -t \\
-t & -t & \epsilon & -t & -t & -t \\
-t & -t & -t & \epsilon & -t & -t \\
-t & -t & -t & -t & \epsilon & -t \\
-t & -t & -t & -t & -t & \epsilon
\end{array}$$

(a)

$$\begin{array}{cccccccccccccccc}
\epsilon & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & \epsilon & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & \epsilon & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & \epsilon & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & \epsilon & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 1 & \epsilon & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 1 & \epsilon & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 1 & \epsilon & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & \epsilon & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & \epsilon & 1 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & \epsilon & 1 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & \epsilon & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & \epsilon & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & \epsilon & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & \epsilon & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & \epsilon
\end{array}$$

(b)

FIGURE 1. The matrix elements for the infinite-range hopping approximation. The example is for six sites. The rows and columns are labeled by the position sites $\mid i \succ$. b) The matrix elements for the infinite dimension approximation (2-d example for 4 sites). The rows and columns are labelled as before.

unphysical feature can be relaxed in further studies taking the t parameter from some random distribution. Volhard's *et al.* [2] scaling is different but the picture of the model is also different as can be seen writing down the matrix elements. This latter model is called of infinite dimension, having connections only to nearest neighbors in each dimension but with an infinite number of them. Our matrix is complete with all the off-diagonal sites taking the t value. Volhard's *et al.*, matrix is of "fractal" design as has been studied by us previously [4]. It has zeroes in some of the off-diagonal terms. We give a picture of both matrices in Figs. 1a and 1b, respectively. We think it is the first time that such a clear difference between the infinite dimension and infinite range approximation is stated.

Volhard's *et al.*, model has been adopted for fermions where promising studies give a new and "local" picture of the Hubbard and other models of strong correlation.

Our original attempt with the infinite-hopping model was applied to a Hartree-Fock term of a negative U Hubbard model with disorder incorporated which led to a very interesting phase diagram for the localized superconductivity phenomenon [1]. We are still exploring the connection of these results with the phenomenology of high-T_c samples [5].

We will discuss in this report a completely new and intuitive solution of the infinite-range Hamiltonian with binary-alloy disorder.

2. THE HAMILTONIAN

The Hamiltonian reads

$$H = -t \sum_{i,j} c_i^\dagger c_j + \sum_i \epsilon_i' c_i^\dagger c_i, \tag{1}$$

where t is the hopping connection with all the sites and ϵ_i which is $\epsilon_i' + t$ includes the diagonal energies with the added diagonal hopping term.

The ϵ_i' are random energies. In particular we think here of the binary alloy case so

$$\begin{aligned} \epsilon_i &= \epsilon_A, \quad \text{with } n_A \text{ terms}, \\ \epsilon_i &= \epsilon_B, \quad \text{with } n_B \text{ terms}, \end{aligned} \tag{2}$$

where $n_A + n_B = N$. There is a certain number of ϵ_A energies and ϵ_B energies completing the total number of degrees of freedom N.

We choose a certain state in position representation formed by the creation operator for an electron having the diagonal energy ϵ_A. We take it as an origin for the atoms of type A, in number n_A and represent it by $|A_0\succ \in n_A$ (where n_A are the atoms of type A). We then propose the following [6] "traslational states"

$$\|A_0\succ - |A_l\succ\succ \tag{3}$$

$l \neq 0$, $l \in n_A$, and analogously for the B cluster

$$\|B_0\succ - |B_l\succ\succ \tag{4}$$

$l \neq 0$, $l \in n_B$.

We call them "traslational states" as they are the difference between two electrons in different position sites.

These $(N-2)$ "traslational states" diagonalize the Hamiltonian

$$H|A_l'\succ = \epsilon_A'\|A_0\succ - |A_L\succ\succ, \qquad l \neq 0,\ l \in n_A, \tag{5}$$

$$H|B_l'\succ = \epsilon_B'\|B_0\succ - |B_l\succ\succ, \qquad l \neq 0,\ l \in n_B. \tag{6}$$

Explicit operator procedure shows:

$$t\sum_{i_j} c_i^\dagger c_j c_l^\dagger |0\succ = -t\sum_{i_j} c_i^\dagger \left[\delta_{j_l} - c_l^\dagger c_j\right]|0\succ = -t\sum_i c_i^\dagger |0\succ, \tag{7}$$

$$\sum_i \epsilon_i c_i^\dagger c_i c_l^\dagger |0\succ = \sum_i \epsilon_i' c_i^\dagger \left[\delta_{i_l} - c_l^\dagger c_i\right]|0\succ = \epsilon_l' c_l^\dagger |0\succ . \tag{8}$$

In order to find the rest of the states we again postulate "cluster states" or "reservoir states."

We call them by these names as they are states that gather all the electrons of type A in one of the states and all those of type B in the other state and they in some sense resemble the Fermi sea of electrons of each type.

$$\begin{aligned} |A\succ &= \sum_{n_A} |c_{l_A}^\dagger\succ, \\ |B\succ &= \sum_{n_B} |c_{l_B}^\dagger\succ . \end{aligned} \tag{9}$$

We look for the linear combinations which are eigenstates. We apply H on the states

$$H|A\succ = (\epsilon_A + t)\,|A\succ - tn_A|A\succ - tn_B|B\succ, \tag{10}$$

$$H|B\succ = (\epsilon_B + t)\,|B\succ - tn_B|B\succ - tn_A|A\succ . \tag{11}$$

The explicit eigenstates in a 2×2 space are:

$$(\omega - \epsilon''_A)\,|A\succ + t_B|B\succ = 0, \tag{12}$$

$$(\omega - \epsilon''_B)\,|B\succ + t_A|A\succ = 0, \tag{13}$$

where the parameters read

$$\epsilon''_A = \epsilon_A + t\,(1 - n_A)\,, \tag{14}$$

$$\epsilon''_B = \epsilon_B + t\,(1 - n_B)\,, \tag{15}$$

$$t_A = t n_A, \tag{16}$$

$$t_B = t n_B. \tag{17}$$

We build the determinantal equation

$$(\omega - \epsilon''_A)\,(\omega - \epsilon''_B) - t_A t_B = 0. \tag{18}$$

Then,

$$\omega = \frac{\epsilon''_A + \epsilon''_B}{2} + \frac{1}{2}\sqrt{(\epsilon''_a - \epsilon''_B)^2 + 4 t_A t_B}. \tag{19}$$

We have therefore solved the infinite-range hopping binary alloy problem. We find:

1. "Traslational states" in number $N-2$ which are localized (without dispersion in the hopping t) which read $\|A_0\succ - |A_l\succ\succ$ with the eigenvalue ϵ'_A and $\|B_0\succ - |B_L\succ\succ$ with the eigenvalue ϵ'_B.
2. The "cluster states" which read: $|A\succ = \sum_{n_A} |c^{\dagger}_{l_A}\succ$ and $|B\succ = \sum_{n_B} |c^{\dagger}_{l_B}\succ$ with the dispersion relation given above.

Now we want to justify our procedure by the precise determinantal rules for the Hamiltonian in the matrix form.

3. THE DETERMINANTAL STUDY

Due to the current interest in matrix manipulations we want to rederive the previous results through explicit and well known mathematical rules for the determinants. We hope not to be too repetitive with this but in our opinion it is interesting to see step by step how the matrix is being diagonalized.

In all that follows in this paragraph we are thinking of the eigenvalue matrix $\omega - H$ where ω has been omitted for clearer visualizations of the matrix parameters.

We choose a finite sample with $n_A = 4$ and $n_B = 5$. The matrix elements read

$$\begin{array}{ccccccccc}
\epsilon_A & -t & -t & -t & -t & -t & -t & -t & -t \\
-t & \epsilon_A & -t & -t & -t & -t & -t & -t & -t \\
-t & -t & \epsilon_A & -t & -t & -t & -t & -t & -t \\
-t & -t & -t & \epsilon_A & -t & -t & -t & -t & -t \\
-t & -t & -t & -t & \epsilon_B & -t & -t & -t & -t \\
-t & -t & -t & -t & -t & \epsilon_B & -t & -t & -t \\
-t & -t & -t & -t & -t & -t & \epsilon_B & -t & -t \\
-t & -t & -t & -t & -t & -t & -t & \epsilon_B & -t \\
-t & -t & -t & -t & -t & -t & -t & -t & \epsilon_B
\end{array} \tag{20}$$

The labels of the rows and columns are $|0_A\succ \ldots |3_A\succ$, $|0_B\succ \ldots |4_B\succ$.

By using the rule that the determinant of the matrix does not change if we sum or substract rows or columns, we first form

$$\begin{array}{ccccccccc}
\epsilon_A & -t-\epsilon_A & -t-\epsilon_A & -t-\epsilon_A & -t & 0 & 0 & 0 & 0 \\
-t & \epsilon_A+t & 0 & 0 & -t & 0 & 0 & 0 & 0 \\
-t & 0 & \epsilon_A+t & 0 & -t & 0 & 0 & 0 & 0 \\
-t & 0 & 0 & \epsilon_A+t & -t & 0 & 0 & 0 & 0 \\
-t & 0 & 0 & 0 & \epsilon_B & -t-\epsilon_B & -t-\epsilon_B & -t-\epsilon_B & -t-\epsilon_B \\
-t & 0 & 0 & 0 & -t & \epsilon_B+t & 0 & 0 & 0 \\
-t & 0 & 0 & 0 & -t & 0 & \epsilon_B+t & 0 & 0 \\
-t & 0 & 0 & 0 & -t & 0 & 0 & \epsilon_B+T & 0 \\
-t & 0 & 0 & 0 & -t & 0 & 0 & 0 & \epsilon_B+t\,,
\end{array} \tag{21}$$

where the row labels of the matrix are:$|0_A\succ$, $|1_A-0_a\succ$, ... , $|3_A-0_A\succ$, $|0_b\succ$, $|1_B-0_b\succ$ ... $|4_B-0_B\succ$. We have substracted the $|0_A\succ$ column from all the A states and the $|0_B\succ$ column from the B states.

Next we add all the A rows with the first A row and all the B rows to the first B row

$$\begin{array}{ccccccccc}
\epsilon_A-3t & 0 & 0 & 0 & -4t & 0 & 0 & 0 & 0 \\
-t & \epsilon_A+t & 0 & 0 & -t & 0 & 0 & 0 & 0 \\
-t & 0 & \epsilon_A+t & 0 & -t & 0 & 0 & 0 & 0 \\
-t & 0 & 0 & \epsilon_A+t & -t & 0 & 0 & 0 & 0 \\
-5t & 0 & 0 & 0 & \epsilon_B-4t & 0 & 0 & 0 & 0 \\
-t & 0 & 0 & 0 & -t & \epsilon_B+t & 0 & 0 & 0 \\
-t & 0 & 0 & 0 & -t & 0 & \epsilon_B+t & 0 & 0 \\
-t & 0 & 0 & 0 & -t & 0 & 0 & \epsilon_B+t & 0 \\
-t & 0 & 0 & 0 & -t & 0 & 0 & 0 & \epsilon_B+t.
\end{array} \tag{22}$$

The column labels are $|0_A\succ + |\sum_i n_i^A\succ$, $|1_A\succ \ldots |3_A\succ$, $|0_B\succ + |\sum_i n_i^B\succ$, $|1_B\succ$ ... $|4_B\succ$.

Rearranging we get

$$\begin{array}{ccccccccc}
\epsilon_A - 3t & -4t & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-5t & \epsilon_B - 4t & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-t & 0 & \epsilon_A + t & 0 & 0 & 0 & 0 & 0 & 0 \\
-t & 0 & 0 & \epsilon_A + t & 0 & 0 & 0 & 0 & 0 \\
-t & 0 & 0 & 0 & \epsilon_A + t & 0 & 0 & 0 & 0 \\
-t & 0 & 0 & 0 & 0 & \epsilon_B + t & 0 & 0 & 0 \\
-t & 0 & 0 & 0 & 0 & 0 & \epsilon_B + t & 0 & 0 \\
-t & 0 & 0 & 0 & 0 & 0 & 0 & \epsilon_B + t & 0 \\
-t & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \epsilon_B + t.
\end{array} \tag{23}$$

The row labels are $|0_A\succ$, $|0_B\succ$, $|1_A - 0_B\succ \ldots |3_A - 0_A\succ$, $|1_B - 0_B\succ \ldots |4_B - 0_B\succ$. The column labels are $|0_A + \sum_i n_i^A\succ, |0_B + \sum_i n_i^B\succ, |1_A\succ \ldots |3_A\succ, |1_B\succ, \ldots |4_B\succ$. Now we expand the determinant along the first row

$$(\epsilon_A - 3t)(\epsilon_B - 4t)(\epsilon'_A)^{n_A-1}(\epsilon'_B)^{n_B-1} - (-5t)(-4t)(\epsilon'_A)^{n_A-1}(\epsilon'_B)^{n_B-1} = 0. \tag{24}$$

Throughout this determinantal presentation we kept in mind of the eigenvalue equation, ω was not written for graphical simplicity of the presentation. Therefore the diagonal elements in all th section should read $\omega - \epsilon$. Putting it now explicitely we have to solve

$$[\omega - (\epsilon_A - 2t)][\omega - (\epsilon_B - 3t)] - (-5t)(-4t) = 0\ . \tag{25}$$

Generalizing

$$\{\omega - [\epsilon_A + (1 - n_A)t]\}\{\omega - [\epsilon_B + (1 - n_B)t]\} - t^2 n_A n_B = 0, \tag{26}$$

we obtain the same result as by the intuitive guess described at the beginning.

We think that this example shows clearly the way of manipulating the matrix in tight-binding models.

In particular for one impurity with the hopping term in the "infinite hopping" approximation we get

$$(\omega - \epsilon_A)\{\omega - [\epsilon_B + (1 - n_B)t]\} - t^2 n_B = 0. \tag{27}$$

4. SCALING

In order to get results in the thermodynamic limit we have to scale the hopping term t with t/N, where $N = n_A + n_B$ is the total number of elements in the alloy so as to get an analytic dependence for the concentration. For example the equation for the "reservoir states" will read

$$\{\omega - [\epsilon_A + (1/N - c_A)t']\}\{\omega - [\epsilon_B + (1/N - c_B)t']\} - (t')^2 c_A c_B = 0, \tag{28}$$

where t' is the bare hopping parameter and $c_{A,B}$ is the respective concentration.

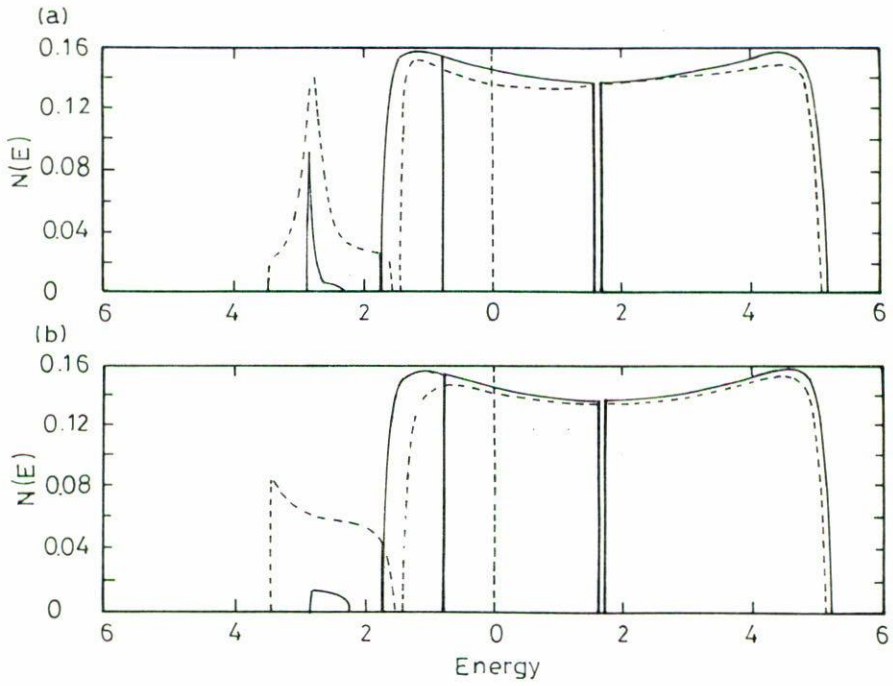

FIGURE 2. a) Density of states for diagonal disorder ($t = 1$) in the case $\epsilon_A = -\epsilon_B = -1.7$ and $c = 0.01$ (full curve) and $c = 0.1$ (broken curve) corresponding to the method of Ref. [8] for a Bethe lattice with coordination number equal to 4. The vertical lines mark the positions of the Delta peaks of the present model (which are almost coincident for both concentrations). b) The same as above for the CPA result.

In order to show more explicitly the result of the infinite-range hopping approximation for binary alloys we plot our points for the results shown in a recent paper [8] as given in Figs. 2a and 2b. In Fig. 2a the authors [8] show the results of their method for two different concentrations of diagonal disorder applied to the Bethe-lattice of coordination number equal to 4. Our scaling results do not distinguish, on the scale of the figure, between the two concentrations. In Fig. 2b the comparison with the coherent potential approximation (CPA) is made. Both of these approximations are for the nearest-neighbors hopping in rather a low dimension so they are essentially different from the infinite range approximation. which has an infinite coordination number. Nevertheless we think it is of interest to compare the results. The infinite dimension approximation as shown by Volhard *et al.*, agrees with the CPA The infinite range hopping result gives a kind of "center of mass" result relative to the nearest-neighbor results for low dimension at least in the approximation available here. It allows to visualize the meaning of the results of the infinite range-hopping approximation with respect to the model most currently thought as representative of the physical solid. Unpublished studies of the Hubbard model made by us along the lines of this paper seem to show that the infinite range approximation picks up special points of the density of states related to the peak, but not exactly the maximum.

The no-disorder limit is reproduced by our exact result. This limit, taking $\epsilon_A = \epsilon_B = 0$, and using the properties for the delta functions, gives for the infinite range hopping approximation the eigenvalue located at the value of the hopping t. In our solution the four delta eigenvalues reduce to t also as can be checked on the formulae of the first section.

The previous comparison with the CPA and with the Bethe-lattice of low coordination number (4) can be seem slightly unnecessary since the connectivities are very different. However since they were available we decided to show them, as to situate the infinite-range approximations with respect to the more realistic ones.

The result for the Bethe lattice with z infinite and nearest-neighbor hopping $t = t/\sqrt{z}$ were given (Ref. [9]). The semicircular density of states is obtained in this case [10]:

$$D(\epsilon) = \frac{1}{2\pi t^2}\sqrt{4t^2 - \epsilon^2}|\epsilon| \prec 2t. \tag{29}$$

We see therefore that the no disorder limit of our approximation gives a degenerate delta function at t whereas the infinite dimension result is the semicircular band extending from $-2t$ to $2t$.

It must not be surprising that although the $\sqrt{z}$ scaling gives bands the z scaling gives deltas as they are very different as shown here.

The closer connection with the original Sherrington-Kirkpatrick problem is not obvious for us at the moment. Perhaps by using the scheme of Volhard *et al.*, one could try a solution of the Wigner-Jordan transformation but we leave it for another work.

5. CONCLUSIONS

We have solved the "infinite range" hopping model with binary alloy disorder by intuition [7] and by the strict determinantal rules applied to the corresponding tight-binding matrix. It is a completely new solution an the eigenstates are not trivial. We find $N-2$ states, where the t term shifts the diagonal energies of the pure alloy only slightly in the thermodynamic limit. They are formed by a difference of two local states inside each cluster. Besides, two reservoir states appear which can be called extended because they have some dependence in the hopping.

Recently Vlaming and Volhardt studied [7] the "infinite dimension" approximation with random diagonal energies using the diagrammatic technique. They find that the density of states is that of the coherent potential approximation (CPA). This approximation gives broad, continuous densities of states.

We find here, with the infinite range hopping approximation, well defined and discrete eigenstates. We show that for our approximation the scaling of t' is t'/Z or t'/N which is the same in our model [1].

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