The extended Heine–Stieltjes polynomials associated with a special LMG model

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Abstract
The extended Heine–Stieltjes polynomials associated with a special Lipkin–Meshkov–Glick (LMG) model corresponding to the standard two-site Bose–Hubbard model are derived based on the Stieltjes correspondence. It is shown that there is a one-to-one correspondence between zeros of this new polynomial and solutions of the Bethe ansatz equations for the LMG model. A one-dimensional classical electrostatic analog corresponding to the special LMG model is established according to Stieltjes’ early work. It shows that any possible configuration of equilibrium positions of the charges in the electrostatic problem corresponds uniquely to one set of roots of the Bethe ansatz equations for the LMG model, and the number of possible configurations of equilibrium positions of the charges equals exactly the number of energy levels in the LMG model. Some relations of sums of powers and inverse powers of zeros of the new polynomials related to the eigenenergies of the LMG model are derived.

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1. Introduction
It is well known from a number of studies [1–3] that the Lipkin–Meshkov–Glick (LMG) model [4–6] has a rich phase structure that is related to a broad range of phenomena in a variety of physical applications, such as analyses of spin systems [7], Bose–Einstein condensates [8], etc. Furthermore, it has been proven [9, 10] that the model is exactly solvable. A special case of the theory is related to the standard two-site Bose–Hubbard model [11] with a Hamiltonian that is equivalent to that of a paramagnet of the easy-axis type in a transverse magnetic field [12]. The quantum dynamics and energy gap of the model were studied in [13, 14]. The quantum critical behavior and a special case of the model were discussed in [15, 16]. As shown in [9–11, 12–16], exact solutions of the model can be determined using the Gaudin–Richardson
or Bethe ansatz method, in which eigenstates of the system are written in terms of a product of spectral parameter-dependent operators. The unknown spectral parameters must satisfy a set of coupled nonlinear equations, called the Bethe ansatz equations (BAEs). Solutions of the BAEs simultaneously determine the eigenenergies and the corresponding eigenstates [9–11].

It should be noted that according to the early work of Stieltjes [17–20] there is an important one-to-one correspondence between every set of BAEs and a set of orthogonal polynomials. And furthermore, as shown by Szegő [21], the Stieltjes correspondence can be used to define a large class of classical orthogonal polynomials. Roots of these BAEs are zeros of the corresponding polynomials, which can be interpreted as stable equilibrium positions for a set of free charges in an external electrostatic field. This link between Richardson’s BCS pairing model for nuclei and the corresponding electrostatic problem was established in [22] based on an earlier unpublished preprint of Gaudin, which was then made clearer in [23]. A much more general approach to the pairing model was shown in [24] and [25]. The purpose of this paper is to show that the Stieltjes correspondence related to the solutions of a special LMG model corresponding to the standard two-site Bose–Hubbard model gives rise to a new polynomial, which is now called the extended Heine–Stieltjes polynomial.

2. Stieltjes correspondence

There is a large class of polynomials, called Heine–Stieltjes polynomials $y(z)$, which satisfy a second-order Fuchsian equation

$$A(x)y''(x) + B(x)y'(x) + V(x)y(x) = 0,$$

where $A(x)$ is a polynomial of degree $m$ with $A(x) = \prod_{i=1}^{m} (x - a_i)$, $B(x)$ is a polynomial of degree $m - 1$ such that for a set of real positive parameters $\gamma_i$ and another set of real parameters $\alpha_i$

$$B(x)/A(x) = \sum_{i=1}^{m} \frac{\gamma_i}{x - \alpha_i},$$

and $V(x)$ is an unknown, but to be determined polynomial of degree $m - 2$ that is allowed to depend on the solution $y(x)$. The latter are often called Van Vleck polynomials [26]. The case with $m = 2$ corresponds to the hypergeometric differential equation, while the case with $m = 3$ corresponds to the Heun equation [27, 28].

Such Heine–Stieltjes polynomials and properties of their zeros have been studied extensively. If the polynomials $A(x)$ and $B(x)$ are algebraically independent, i.e. they do not satisfy any algebraic equation with integer coefficients, Heine proved that for every integer $k$ there exist at most $\sigma(k) = (k + m - 2)!/(m - 2)!k!$ different Van Vleck polynomials $V(x)$ such that $y(x)$ has a polynomial solution of degree $k$. As summarized in Szegő’s work on orthogonal polynomials [21], for every set of nonnegative integers $(k_1, k_2, \ldots, k_m)$, there are uniquely determined real values of the parameters for the Van Vleck polynomials $V(x)$ such that $y(x)$ has a polynomial solution with $k_j$ simple zeros in the open interval $(a_{j-1}, a_j)$ for each $j = 1, 2, \ldots, m$. The polynomial $y(x)$ is uniquely determined up to a constant factor, and has the degree $k = k_1 + \cdots + k_m$. As noted by Volkmer [29], this existence and uniqueness theorem can also be derived from the general Klein oscillation theorem for multi-parameter eigenvalue problems shown in [30].

If $y(x)$ is a polynomial of degree $k$ with simple zeros $\{x_1, x_2, \ldots, x_k\}$, one may write $y(x)$ as

$$y(x) = \prod_{j=1}^{k} (x - x_j).$$
Thus, one can easily check that \( y(x) \) will satisfy
\[
y''(x_i) = \sum_{j \neq i} \frac{2}{x_i - x_j}
\] at any zero \( x_i \). Combining (1), (2) and (4), one obtains the following important relations among the zeros:
\[
\sum_{j \neq i} \frac{2}{x_i - x_j} + \sum_{\mu=1}^{m} \frac{Y_\mu}{x_i - a_\mu} = 0
\]
for \( i = 1, 2, \ldots, k \). It should be noted that the BAEs frequently appearing in search for exact solutions of quantum many-body problems, such as those associated with Gaudin-type systems, are similar to the relations shown in (5). The link between Richardson’s BCS pairing model for nuclei and the corresponding electrostatic problem was investigated in [22] based on an earlier unpublished preprint of Gaudin, which was then made clearer in [23]. A much more general approach to the pairing model was shown in [24] and [25]. Roots of the BAEs (5) simultaneously determine the eigenenergies and eigenstates of the corresponding quantum many-body problem. As an alternative, roots of the BAEs may also be calculated as zeros of the corresponding polynomial \( y(x) \). In this way, a link between solutions of the Gaudin type for quantum many-body problems and the corresponding polynomials is established.

3. Special LMG model and Bethe ansatz solutions

As a simple extension of the Stieltjes correspondence, we revisit the Bethe ansatz solutions for a special LMG model corresponding to the standard two-site Bose–Hubbard model studied in [11, 13–15], for which the Hamiltonian is
\[
\hat{H} = -t (c^\dagger d + d^\dagger c) + U (c^\dagger cc^\dagger c + d^\dagger dd^\dagger d),
\]
where \( c^\dagger (c) \) and \( d^\dagger (d) \) are boson creation (annihilation) operators; the parameters \( t \) and \( U \) in the Bose–Hubbard model are related to the Josephson coupling and the charging energy, respectively. Following [11, 15], we use the unitary transformation for the boson operators with
\[
c = \sqrt{\frac{1}{2} (a - ib)}, \quad d = \sqrt{\frac{1}{2} (a + ib)}.
\]
Then, the Hamiltonian (6) can be rewritten in terms of \( a \)- and \( b \)-boson operators as
\[
\hat{H} = t (b^\dagger b - a^\dagger a) - \frac{1}{2t} U S^+(0) S^- (0) + U \hat{n}^2,
\]
where \( \hat{n} = a^\dagger a + b^\dagger b \) is the operator for the total number of bosons in the system, and
\[
S^+(0) = b^\dagger^2 + a^\dagger^2, \quad S^- (0) = b^2 + a^2
\]
are boson pairing operators.

Let \( |v_1, v_2\rangle = a^{v_1} b^{v_2} |0\rangle \) with \( v_i = 0 \) or 1 for \( i = 1, 2 \) be the \( a \)- and \( b \)-boson pairing vacuum state satisfying
\[
a^2 |v_1, v_2\rangle = b^2 |v_1, v_2\rangle = 0.
\]
To diagonalize the Hamiltonian, we use the algebraic Bethe ansatz which implies that eigenvectors of (8) may be expressed as
\[
|n, \zeta, v_1, v_2\rangle = S^+(x_1^{(C)}) S^+(x_2^{(C)}) \cdots S^+(x_k^{(C)}) |v_1, v_2\rangle
\]
with \( n = 2k + v_1 + v_2 \), and
\[
S^+(x_i^{(\nu)}) = \frac{a^{i2}}{x_i^{(\nu)} + 1} + \frac{b^{i2}}{x_i^{(\nu)} - 1},
\]
for \( i = 1, 2, \ldots, k \). in which \( x_i^{(\nu)} \) (\( i = 1, 2, \ldots, k \)) are spectral parameters to be determined, and \( \zeta \) is an additional quantum number for distinguishing different eigenvectors with the same quantum number \( k \). It can then be verified by using the corresponding eigenequation that (11) is a solution when the spectral parameters \( x_i^{(\nu)} \) (\( i = 1, 2, \ldots, k \)) satisfy the following set of BAEs:
\[
U \left( \frac{2v_1 + 1}{x_i^{(\nu)} + 1} + \frac{2v_2 + 1}{x_i^{(\nu)} - 1} \right) + 2t + 4U \sum_{j \neq i} \frac{1}{x_i^{(\nu)} - x_j^{(\nu)}} = 0
\]
for \( i = 1, 2, \ldots, k \), with the corresponding eigenenergy given by
\[
E_{\alpha}^{(\nu)} = 2t \sum_{i=1}^{k} x_i^{(\nu)} + t(v_2 - v_1) + Un^2.
\]
Hence, once the \( \zeta \)-th roots \( \{x_i^{(\nu)}\} \) are obtained from equation (13), the eigenenergy and the corresponding eigenstate are thus determined according to (14), (11) and (12).

4. The extended Heine–Stieltjes polynomials associated with solutions of the LMG model

In order to compare to the Stieltjes correspondence, we assume \( t > 0 \) and \( U \neq 0 \), and set
\[
\alpha = v_1 + 1/2, \quad \beta = v_2 + 1/2, \quad \gamma = t/U.
\]
Then, the BAEs (13) become
\[
\left( \frac{\alpha}{x_i^{(\nu)} - 1} + \frac{\beta}{x_i^{(\nu)} + 1} \right) + \gamma + \sum_{j \neq i} \frac{2}{x_i^{(\nu)} - x_j^{(\nu)}} = 0.
\]
When \( U > 0 \), all parameters \( \alpha, \beta \) and \( \gamma \) are always positive. When \( U < 0 \), we interchange the boson operator \( a^i \) with \( b^i \) in (12). Then, one can easily verify that such a change is equivalent to interchange \( v_1 \) with \( v_2 \) and \( t \to -t \) in the BAEs (13), which leads to the final BAEs for the \( U < 0 \) case that is the same as (16) with \( \alpha \leftarrow \beta \) and keeping \( \alpha > 0, \beta > 0 \) and \( \gamma > 0 \). Hence, it is sufficient to consider the case for \( U > 0 \) only with BAEs given by (16).

Although the \( \gamma = 0 \) result is trivial for the LMG model, according to the Stieltjes correspondence, the polynomial corresponding to (16) in this case is the Jacobi polynomial \( P_k^{(\alpha-1, \beta-1)}(x) \) satisfying the well-known differential equation
\[
\frac{d^2}{dx^2} P_k^{(\alpha-1, \beta-1)}(x) + \left( \frac{\alpha}{x - 1} + \frac{\beta}{x + 1} \right) \frac{d}{dx} P_k^{(\alpha-1, \beta-1)}(x) - \frac{k(k + \alpha + \beta - 1)}{x^2 - 1} P_k^{(\alpha-1, \beta-1)}(x) = 0.
\]
In this case, the Van Vleck polynomial \( V(x) \) is trivially a \( k \)-dependent constant. Hence, there is only one set of zeros of \( P_k^{(\alpha-1, \beta-1)}(x_i) \) with \( i = 1, 2, \ldots, k \), satisfying the BAE (16).

The case with \( \gamma \neq 0 \) is non-trivial. According to (1)–(5), we write a differential equation corresponding to the BAE (16) as
\[
\frac{d^2y(x)}{dx^2} + \left( \frac{\alpha}{x - 1} + \frac{\beta}{x + 1} + \gamma \right) \frac{dy(x)}{dx} + \frac{V(x)}{x^2 - 1} y(x) = 0
\]
with the corresponding polynomials $A(x) = x^2 - 1$ and $B(x) = \gamma x^2 + (\alpha + \beta)x + \alpha - \beta - \gamma$ shown in (1). In contrast to the Heine–Siltjes equation (1), however, in this case the polynomial $B(x)$ is of the same degree as that of $A(x)$. Therefore, the polynomials $y(x)$ determined by (18) should be similar to but different from those of Heine–Siltjes type.

In the search for polynomial solutions of (18), we write

$$y_k(x) = \sum_{j=0}^{k} b_j x^j. \quad (19)$$

Substitution of (19) into (18) yields the condition to determine the corresponding polynomial $V(x)$ with

$$V(x) = -\gamma kx + f, \quad (20)$$

where $f$ is an undetermined constant depending on $k$, together with the expansion coefficients $b_j$, satisfying the following four-term relations:

$$(j(\alpha + \beta + j - 1) + f)b_j = (j + 2)(j + 1)b_{j+2} + (j + 1)(\beta - \alpha + \gamma)b_{j+1} + \gamma(k - j + 1)b_{j-1} \quad (21)$$

with $b_j = 0$ for $j \leq -1$ or $j \geq k + 1$, which is equivalent to the following eigenequation for $f$ with

$$Fb = \gamma k + f, \quad (22)$$

where

$$F = \begin{pmatrix}
0 & (\beta - \alpha + \gamma) & 2 & 0 & \cdots \\
\gamma & -(\alpha + \beta) & 2(\beta - \alpha + \gamma) & 6 & 0 & \cdots \\
0 & (k - 1)\gamma & -2(\alpha + \beta + 1) & 3(\beta - \alpha + \gamma) & 12 & 0 & \cdots \\
& & & & & \ddots & \ddots & \ddots \\
& & & & & & \ddots & \ddots & \ddots \\
& & & & & & & \ddots & \ddots & \ddots \\
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& & & & & & & & & & & & \ddots & \ddots & \ddots \\
& & & & & & & & & & & & & 2\gamma & -(k - 1)(\alpha + \beta + k - 2) & k(\beta - \alpha + \gamma) \\
& & & & & & & & & & & & & & \gamma & -k(\alpha + \beta + k - 1) 
\end{pmatrix} \quad (23)$$

and the transpose of $b$ is related to the expansion coefficients $\{b_j\}$ with $b^T = (b_0, b_1, \ldots, b_{k-1}, b_k)$. It is clear that the matrix $F$ should have $k + 1$ eigenvalues labeled as $f^{(i)}(\zeta = 1, 2, \ldots, k + 1)$, of which the corresponding eigenvector $b^{(i)}$ determines the polynomial $y^{(i)}_k(x)$ according to (19). The number of solutions for $f$ is indeed the same as that of the eigenstates of the standard two-site Bose–Hubbard Hamiltonian (8) when $\gamma \neq 0$.

The polynomials (19) with $\gamma \neq 0$ determined by (21) are called the extended Heine–Stieltjes polynomials, which, in general, can also be obtained from the Riccati differential equation studied in [31, 32] or from relevant BAEs given in [33] though these authors did not intend to do so. It should be noted that the polynomial approach shown above is similar to that studied in [34–36] for quasi-exactly solvable sextic anharmonic oscillator problem and $PT$-symmetric quantum mechanics. Since the BAEs of the quasi-exactly solvable sextic anharmonic oscillator problem and $PT$-symmetric quantum mechanics are different from those for the special LMG model, the resultants should belong to different types of extended Heine–Stieltjes polynomials.

As is well known, the advantage of the Bethe ansatz method for the Gaudin-type systems lies in the fact that the huge matrix in the Fock subspace is greatly reduced, especially for the Gaudin–Richardson pairing model [22–25]. However, the nonlinear BAEs similar to (16) are very difficult to solve numerically, especially for large size systems. There are several attempts to overcome this difficulty. The approach via the Riccati differential equation shown

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in \([31, 32]\) is one of them. Actually, if the polynomials can be derived recursively similar to (21) for the LMG model, it should be much easier to determine zeros from the polynomials than to solve a set of BAEs with a set of variables because there is only one variable in the polynomials. In order to make this point clear, let us take a simple nontrivial example with \(k = 2\) and \(\alpha = \beta = \gamma = 1/2\) corresponding to \(v_1 = v_2 = 0\) and \(t/U = 1/2\). In this case, the three polynomials \(y_2(x)\) given by (19) with \(b_2 = 1\) can easily be obtained from the four-term recurrence relations (21) as listed in table 1. Since we set \(b_k = 1\) in \(y(x)\), the coefficient \(b_{k-1}\) must be equal to the negative sum of zeros of \(y(x)\) with \(b_{k-1} = -\sum_{i=1}^{k} x_i\). Therefore, the solution corresponding to the largest \(b_{k-1}\) is that for the ground state of the system considered; that corresponding to the next largest \(b_{k-1}\) is that of the first excited state; and so on. One can check that these are indeed the cases as shown in table 1.

According to the Stieltjes results, an electrostatic interpretation of the location of zeros of the new polynomial \(y(x)\) may be stated as follows. Put two positive fixed charges \(\alpha/2\) and \(\beta/2\) at \(-1\) and \(+1\) along a real line, respectively, and allow \(k\) positive unit charges to move freely along the real line under such situation together with a uniform electric field with strength \(-\gamma/2\). Therefore, up to a constant, the total energy functional \(U(x_1, x_2, \ldots, x_k)\) may be written as
\[
U(x_1, x_2, \ldots, x_k) = -\frac{\gamma}{2} \sum_i x_i - \frac{\alpha}{2} \sum_i \ln|x_i - 1| - \frac{\beta}{2} \sum_i \ln|x_i + 1| - \sum_{1 \leq i < j \leq k} \ln|x_i - x_j|.
\]

\[
(24)
\]

In this case, there are \(k + 1\) different configurations for the position of these \(k\) charges \(\{x_1^{(1)}, \ldots, x_k^{(1)}\}\) with \(\xi = 1, 2, \ldots, k + 1\), corresponding to global minimums of the total energy. As proven by Stieltjes, there is a unique configuration with \(-1 < x_1 < \cdots < x_k < 1\) when \(\gamma = 0\) which corresponds to the zeros of the Jacobi polynomial \(P_k^{(\alpha - 1, \beta - 1)}(x)\). When \(\gamma > 0\), however, one can verify numerically, as in [15], that the range of the positions of these positive unit charges tends to be along the entire half line except the two singular points \(\pm 1\) with \(x_1, \ldots, x_k \in (-\infty, -1) \cup (-1, +1)\). Let the positions of these positive charges be arranged as \(x_1 < x_2 < \cdots < x_k\). The above restriction requires that these positions must be within the intervals \((-\infty, -1)\) and \((-1, +1)\) with \(-\infty < x_1 < x_2 < \cdots < x_k < -1 < x_{k+1} < \cdots < x_k < +1\). It follows from this that the total number of possible configurations is exactly the number of ways to put the \(k\) positive charges into the two intervals, which is \((k + m - 1) = k + 1\) for \(m = 2\).

Some explicit formulas for sums of powers of zeros of the new polynomials can easily be derived. For example, summing equation (16) over \(i\), we have
\[
(\alpha - \beta) \sum_{i=1}^{k} \frac{1}{x_i^2 - 1} + (\alpha + \beta) \sum_{i=1}^{k} \frac{x_i}{x_i^2 - 1} = -k\gamma.
\]

\[
(25)
\]

while multiplying equation (16) by \(x_i\) and then summing over \(i\), we obtain
\[
(\alpha + \beta) \sum_{i=1}^{k} \frac{1}{x_i^2 - 1} + (\alpha - \beta) \sum_{i=1}^{k} \frac{x_i}{x_i^2 - 1} + \gamma \sum_{i=1}^{k} x_i = -k(\alpha + \beta + k - 1).
\]

\[
(26)
\]
Equations (25) and (26) can be combined to express $\gamma \sum_{i=1}^{k} x_i$ related to the eigenenergy (14) as

$$\gamma \sum_{i=1}^{k} x_i = \frac{4\alpha\beta}{\alpha + \beta} \sum_{i=1}^{k} \frac{1}{1 - x_i^2} - k \left( \alpha + \beta + k - 1 - \frac{\gamma \alpha - \beta}{\alpha + \beta} \right).$$

(27)

Additional sum rules can be derived from the explicit form of the new polynomial $y_k(x)$ by using the method shown in [37–39] for other polynomials. Let the polynomial $y_k(x)$, up to a constant, be expressed in terms of its zeros as

$$y_k(x) = \prod_{i=1}^{k} (x - x_i).$$

(28)

Then, the expansion coefficients in (19) can be explicitly written as

$$b_k = 1, \quad b_{l-1} = -\sum_{i=1}^{k} x_i, \quad b_{l-2} = \sum_{i<j} x_ix_j, \ldots, b_0 = (-)^k \prod_{i=1}^{k} x_i.$$  \hspace{7cm} (29)

Directly using the four-term relation (21) with the explicit expressions shown in (29), we have, for example,

$$f = \sum_{1 \leq i < j \leq k} 2x_ix_j + (\alpha - \beta - \gamma) \sum_{i=1}^{k} \frac{1}{x_i}$$

$$= \left( \sum_{i=1}^{k} \frac{1}{x_i} \right)^2 - (k-1) \sum_{i=1}^{k} \frac{1}{x_i^2} + (\alpha - \beta - \gamma) \sum_{i=1}^{k} \frac{1}{x_i}$$

(30)

for $k \geq 2$, and

$$f = -\gamma \sum_{i=1}^{k} x_i - k(\alpha + \beta + k - 1),$$

(31)

which provides a relation among the eigenvalues $f$ in the differential equation (18) and the eigenenergies (14) of the special LMG model. Equation (31) can easily be verified from the results shown in table 1.

Sum rules of other higher order powers and inverse powers of zeros of the new polynomials may also be derived from the four-term relation (21) by using explicit expressions shown in (29). Equation (31) clearly shows that $f = -k(\alpha + \beta + k - 1)$ corresponding to the Jacobi polynomial with $y_k(x) = P_k^{(\alpha-1, \beta-1)}(x)$ when $\gamma = 0$.

5. Summary and discussions

In this paper, new polynomials, similar to but distinct from those of the Heine–Stieltjes type, that are associated with a special LMG model corresponding to the standard two-site Bose–Hubbard model are derived based on the Stieltjes correspondence. It follows that the eigenvalues and corresponding eigenstates of the special LMG model can be determined from the zeros of these polynomials. Further, if these polynomials can be derived recursively, it also follows that it should be much easier to determine zeros from the polynomials, e.g. the case considered in [40], than to solve a set of BAEs with a set of variables because there is only one variable in the polynomials. This conclusion applies equally well to other quantum many-body systems, such as atomic-molecular Bose–Einstein condensates [41], the heteronuclear molecular Bose–Einstein condensate model [42] and the nuclear pairing problem, when the corresponding polynomials can be obtained. It is well known that the Jacobi polynomials
$P^{(α, β)}_k(x)$ are orthogonal with respect to the measure $dμ(x) = (x−1)^α(x+1)^β \, dx$ on the interval $x ∈ (−1, +1)$. Although the orthogonality of the new polynomials is not addressed, we conjecture that, similar to the Lamé polynomials analyzed in [43, 44], there is no sequence of the new polynomials orthogonal with respect to any measure supported on the interval $(−∞, 1)$ when $γ ≠ 0$. A rigorous proof of the latter, which requires further work, is beyond the scope of this study. Furthermore, following Stieltjes’ early work, a one-dimensional classical electrostatic analog corresponding to the special LMG model is established. This shows that any possible configuration of equilibrium positions of the charges in the electrostatic problem corresponds uniquely to one set of roots of the BAEs for the LMG model, and that the number of possible configurations of equilibrium positions of the charges equals exactly to the number of energy levels in the LMG model. Sum rules of powers and inverse powers of zeros of the new polynomials related to eigenenergies of the LMG model are also considered. More complicated sum rules and their relations may be obtained similarly. The results by extension clearly show a new link between Bethe ansatz-type solutions of large class of quantum many-body problems and a class of polynomials satisfying second-order differential equations, and thus opens a new way to obtain solutions of these BAEs from zeros of these polynomials.

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