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# Sum rules for harmonic-oscillator brackets†

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**Abstract.** A new class of sum rules is derived for the coefficients of the Talmi transformation of the harmonic-oscillator wavefunctions from the single particle coordinates to the relative and the centre-of-mass coordinates.

## 1. Introduction

It is well known that harmonic-oscillator wavefunctions (HOWF) have the property that a product of two wavefunctions can be transformed from the single-particle coordinates to the relative and the centre-of-mass coordinates (Talmi 1952). This is known as the Talmi transformation and the transformation coefficients are called the oscillator brackets or the Talmi–Brody–Moshinsky (TBM) coefficients (Moshinsky 1959, Brody and Moshinsky 1967). This transformation simplifies the calculation of two-body matrix elements and the coefficients are widely used in nuclear structure calculations (de-Shalit and Talmi 1963). Various methods for the calculation of these coefficients and several explicit expressions for the coefficients are described in the literature (Trlifaj 1972 and references therein). The brackets satisfy the standard orthogonality relations and have some simple symmetries. In this work I derive a class of sum rules for the HO brackets, which are independent of the orthogonality relations. Some of the sum rules are due to the well known symmetry properties of the HO brackets but others are new relations. These new relations demonstrate interesting properties of the HO brackets. Of course, one may use the sum rules to derive an expression for (and to calculate) the HO brackets. However, since there exist in the literature several codes for the evaluation of the HO brackets, the sum rules are particularly useful in providing an independent check for the results of these codes.

## 2. Derivation of the sum rules

### 2.1. The one-dimensional case

Let us first consider the one-dimensional case. The harmonic-oscillator (HO) Hamiltonian can be written in the form

$$H=\tfrac{1}{2}(p^2+x^2)\hbar\omega, \tag{1}$$

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where $p$ and $x$ are in units of $\hbar\sqrt{\nu}$ and $1/\sqrt{\nu}$, respectively, and $\nu = m\omega/\hbar$. The eigenvalues of (1) are of the form $(K+\frac{1}{2})\hbar\omega$, where $K$ is a positive integer; the corresponding eigenfunctions are

$$\psi_K(x) = (\sqrt{\pi}2^K K!)^{-1/2} e^{-x^2/2} H_K(x), \tag{2}$$

where $H_K(x)$ is the Hermite polynomial,

$$H_K(x) = K! \sum_{m=0}^{[K/2]} (-1)^m \frac{(2x)^{K-2m}}{m!(K-2m)!}. \tag{3}$$

Here $[K/2]$ equals $K/2$ or $(K-1)/2$ if $K$ is even or odd, respectively. The HO brackets $\langle kK|K_1K_2\rangle$ are defined by

$$\psi_{K_1}(x_1)\psi_{K_2}(x_2) = \sum_{k+K=K_1+K_2} \langle kK|K_1K_2\rangle \psi_k(x)\psi_K(X), \tag{4}$$

where $x$ is the relative coordinate and $X$ is the centre-of-mass coordinate, given by

$$x = (x_1 - x_2)/\sqrt{2}, \qquad X = (x_1 + x_2)/\sqrt{2}. \tag{5}$$

Using (2) to (5), one finds that (Chasman and Wahlborn 1967)

$$\langle kK|K_1K_2\rangle = \left(\frac{k!K!}{K_1!K_2!}\right)^{1/2} 2^{-(K_1+K_2)/2} \sum_n (-1)^n \binom{K_1}{k-n}\binom{K_2}{n}. \tag{6}$$

The HO brackets (6) obey the orthogonality relations and the symmetry relations

$$\langle kK|K_1K_2\rangle = (-1)^k \langle kK|K_2K_1\rangle = (-1)^{K_2}\langle Kk|K_1K_2\rangle. \tag{7}$$

To derive the sum rules for the HO brackets, I first Fourier transform (4) over the relative coordinate $x$. This is also known as the Wigner transform (Wigner 1932). One can utilise the Rodrigues formulae for the Hermite and the associated Laguerre polynomials (Magnus *et al* 1966) to carry out the Wigner transform of the left-hand side (LHS) and obtain (Bartlett and Moyal 1949)

$$\begin{aligned} f_{K_1K_2}(x,p) &\equiv \frac{1}{2\pi}\int_{-\infty}^{\infty} ds\, e^{ips}\psi^*_{K_1}(x+s/2)\psi_{K_2}(x-s/2) \\ &= \frac{(-1)^{K_2}}{\pi}\left(\frac{K_2!}{K_1!}\right)^{1/2} 2^{(K_1-K_2)/2} e^{-(x^2+p^2)}((x+ip)^{K_1-K_2} L_{K_2}^{K_1-K_2}(2x^2+2p^2), \end{aligned} \tag{8}$$

where $L_K^\alpha(x)$ is the associated Laguerre polynomial,

$$L_K^\alpha(x) = \sum_{l=0}^{K} \binom{K+\alpha}{K-l} \frac{(-1)^l x^l}{l!}. \tag{9}$$

Substituting (9) in (8) and using

$$\sum_n (-1)^n \binom{K_1-K_2}{N-2n}\binom{K_2}{n} = \sum_n (-1)^n \binom{K_1}{N-n}\binom{K_2}{n}, \tag{10}$$

together with (6) and (7), I find that

$$\begin{aligned} f_{K_1K_2}(x,p) = \frac{1}{\pi} e^{-(x^2+p^2)} \sum_{N,M} C_{NM}^{K_1K_2} \\ \times \langle NM|\tfrac{1}{2}(N+M+K_1-K_2)\tfrac{1}{2}(N+M-K_1+K_2)\rangle(2ip)^N(2x)^M, \end{aligned} \tag{11}$$

where the coefficient $C$ is defined by

$$1/C_{NM}^{K_1K_2} = (-1)^{(K_1+K_2-N-M)/2}[\tfrac{1}{2}(K_1+K_2-N-M)]!\times\left(\frac{N!M!}{K_1!K_2!}[\tfrac{1}{2}(N+M+K_1-K_2)]![\tfrac{1}{2}(N+M-K_1+K_2)]!\right)^{1/2}. \quad (12)$$

The sum in (11) is limited by $|K_1-K_2| \leq N+M \leq K_1+K_2$ and $N+M+K_1+K_2$ must be even, i.e. $N+M = |K_1-K_2|, |K_1-K_2|+2, \ldots, K_1+K_2$. Note that in (8) and (11) $f_{K_1K_2}(x,p) = f^*_{K_2K_1}(x,p) = f_{K_2K_1}(x,-p)$. This can be verified using (7) and the fact that $C_{NM}^{K_1K_2}$ in (12) is symmetric under the interchange of $K_1$ and $K_2$ or $N$ and $M$.

Utilising (11) together with the transform

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx\, e^{ipx}\psi_k(x) = i^k\psi_k(p), \quad (13)$$

for the right-hand side (RHS) of (4) I find, using (2), that

$$\sum_{k+K=K_1+K_2} \langle kK|K_1K_2\rangle (k!K!2^{(K_1+K_2)})^{-1/2}\, i^k H_k(\sqrt{2}p)H_K(\sqrt{2}x) = \sum_{NM} C_{NM}^{K_1K_2}\langle NM|\tfrac{1}{2}(N+M+K_1-K_2)\tfrac{1}{2}(N+M-K_1+K_2)\rangle (2ip)^N(2x)^M. \quad (14)$$

Substituting the explicit expression (3) for the Hermite polynomial in (14) and equating the coefficients of $(ip)^N x^M$, I find the sum rule

$$\sum_{k+K=K_1+K_2} \langle kK|K_1K_2\rangle(-1)^{(K-M)/2}(k!K!)^{1/2}\Big/\left[\left(\frac{k-N}{2}\right)!\left(\frac{K-M}{2}\right)!\right] = 2^{(K_1+K_2-N-M)/2}N!M!C_{NM}^{K_1K_2}\langle NM|\tfrac{1}{2}(N+M+K_1-K_2)\tfrac{1}{2}(N+M-K_1+K_2)\rangle, \quad (15)$$

for each pair $(N,M)$ that satisfies $N+M \leq K_1+K_2$ with $N+M+K_1+K_2$ even. The sum over $k$ and $K$ is further limited by the requirements that $k-N$ and $K-M$ are non-negative even integers. It should be noted that for $N+M\langle|K_1-K_2|$, the RHS of (15) vanishes and the sum rule has a simple form.

### 2.2. *The three-dimensional case*

Sum rules for the brackets of a HO of higher dimensions can be derived in a similar way by using the transformation coefficients of the HOWF from the chosen coordinate system to the Cartesian coordinate system. I will now consider in some detail the three-dimensional case in spherical coordinates. In this case $x$ and $p$ in (1) should be replaced by the vectors $\boldsymbol{r} = (x, y, z)$ and $\boldsymbol{p} = (p_x, p_y, p_z)$, respectively. The eigenvalues of the HO Hamiltonian are $E_{nl} = (2n+l+3/2)\hbar\omega$ with the corresponding wavefunctions

$$\psi_{nlm}(\boldsymbol{r}) = U_{nl}(r)Y_{lm}(\theta,\phi), \quad (16)$$

where $Y_{lm}(\theta,\phi)$ are the spherical harmonics and

$$U_{nl}(r) = [2(n!)/\Gamma(n+l+3/2)]^{1/2} r^l e^{-r^2/2} L_n^{l+1/2}(r^2). \quad (17)$$

As before, $r$ is in units of $1/\sqrt{\nu}$. The TBM coefficients $(nlNL\lambda|n_1l_1n_2l_2\lambda)$ are defined by (Brody and Moshinsky 1967)

$$\sum_{m_1+m_2=\mu} \langle l_1m_1l_2m_2|\lambda\mu\rangle\psi_{n_1l_1m_1}(\boldsymbol{r}_1)\psi_{n_2l_2m_2}(\boldsymbol{r}_2)$$
$$= \sum_{nlNL}\sum_{m+M=\mu}(nlNL\lambda|n_1l_1n_2l_2\lambda)\langle lmLM|\lambda\mu\rangle\psi_{nlm}(\boldsymbol{r})\psi_{NLM}(\boldsymbol{R}), \tag{18}$$

where $\boldsymbol{r}=(\boldsymbol{r}_1-\boldsymbol{r}_2)/\sqrt{2}$, $\boldsymbol{R}=(\boldsymbol{r}_1+\boldsymbol{r}_2)/\sqrt{2}$ and $\langle l_1m_1l_2m_2|\lambda\mu\rangle$ is the Clebsch-Gordan coefficient. The sum over $n$, $l$, $N$ and $L$ in (18) is restricted by the energy-conservation condition $2n+l+2N+L=\rho=\rho_1+\rho_2$, where $\rho_1=2n_1+l_1$ and $\rho_2=2n_2+l_2$. The TBM coefficients obey the orthogonality relations and some symmetry relations given by Brody and Moshinsky (1967).

The transformation coefficients $\langle K_1K_2K_3|nlm\rangle$ from the spherical coordinates system to the Cartesian coordinates system are defined by (Chacón and de Llano 1963, Chasman and Wahlborn 1967)

$$\psi_{nlm}(\boldsymbol{r}) = \sum_{K_1+K_2+K_3=2n+l}\langle K_1K_2K_3|nlm\rangle\psi_{K_1}(x)\psi_{K_2}(y)\psi_{K_3}(z), \tag{19}$$

where $\psi_K(x)$ is given by (2). The explicit expression for the coefficient $\langle K_1K_2K_3|nlm\rangle$, the orthogonality relations, and the properties given by Chasman and Wahlborn (1967), will be used in the following. To derive the sum rule for the TBM coefficients I now Fourier transform (18) over the relative coordinate $\boldsymbol{r}$ using (19). This leads to

$$\frac{1}{\pi^{3/2}}\sum_{m+M=\mu}\sum_{nlNL}\langle lmLM|\lambda\mu\rangle(nlNL\lambda|n_1l_1n_2l_2\lambda)\mathrm{i}^{2n+l}\psi_{nlm}(\sqrt{2}\boldsymbol{p})\psi_{NLM}(\sqrt{2}\boldsymbol{R})$$
$$= \sum_{m_1+m_2=\mu}\sum_{K_i,K_i'}\langle l_1m_1l_2m_2|\lambda\mu\rangle\langle K_1K_2K_3|n_1l_1m_1\rangle$$
$$\times\langle K_1'K_2'K_3'|n_2l_2m_2\rangle f_{K_1K_1'}(X,p_x)f_{K_2K_2'}(Y,p_y)f_{K_3K_3'}(Z,p_z), \tag{20}$$

where the sums over $K_i$ and $K_i'$ are limited by $K_1+K_2+K_3=2n_1+l_1$ and $K_1'+K_2'+K_3'=2n_2+l_2$. Equation (20) holds for any value of $n_1$, $l_1$, $n_2$, $l_2$, $\lambda$ and $\mu$. A sum rule is obtained for each set of $(r,s,t,u,v,w)$ by comparing the coefficients of $(\mathrm{i}p_x)^r(\mathrm{i}p_y)^s(\mathrm{i}p_z)^t(X)^u(Y)^v(Z)^w$ of both sides in (20). The general expression of the sum rule for the TBM coefficients is given in the appendix. For special values of $r$, $s$, $t$, $u$, $v$ and $w$, the sum rule can be simplified by employing well known properties of the Clebsch–Gordan coefficients and the transformation coefficients $\langle K_1K_2K_3|nlm\rangle$.

As an example I now discuss the relatively simple results for the case in which $r=s=u=v=0$, i.e. $\boldsymbol{p}=(0,0,p)$ and $\boldsymbol{R}=(0,0,Z)$. In this case $m=M=\mu=0$ in (20). Using (11) for $f$ and (16) and (17) for $\psi_{nl0}$ and $\psi_{NL0}$ in (20) and equating the coefficients of $(\mathrm{i}p)^t(Z)^w$, I obtain the sum rule

$$\sum_{nlNL}\langle l0L0|\lambda\,0\rangle D_{tw}^{nlNL}(nlNL\lambda|n_1l_1n_2l_2\lambda)$$
$$= 2^{(t+w)/2}\langle tw|\tfrac{1}{2}(t+w+\rho_1-\rho_2)\tfrac{1}{2}(t+w-\rho_1+\rho_2)\rangle$$
$$\times\sum_{K_i,K_3'}\sum_{m_1}(-1)^{l_1-m_1}\langle l_1m_1l_2-m_1|\lambda\,0\rangle(-1)^{K_3}C_{tw}^{K_3K_3'}$$
$$\times\langle K_1K_2K_3|n_1l_1m_1\rangle\langle K_1K_2K_3'|n_2l_2m_2\rangle^*, \tag{21}$$

where

$$D_{tw}^{nlNL} = (-1)^{(2n+w-L)/2}\left(\frac{\pi(2l+1)(2L+1)(n!)(N!)}{4\Gamma(n+l+\frac{3}{2})\Gamma(N+L+\frac{3}{2})}\right)^{1/2}$$
$$\times\binom{n+l+\frac{1}{2}}{(2n+l-t)/2}\binom{N+L+\frac{1}{2}}{(2N+L-w)/2}\Big/\left[\left(\frac{t-l}{2}\right)!\left(\frac{w-L}{2}\right)!\right]. \qquad (22)$$

In (21), the sums over $l$ and $L$ are restricted by the requirement that $(t-l)/2$ and $(w-L)/2$ are non-negative integers (see (22)), and the sums over $K_i$ and $K_3'$ are limited by $K_1+K_2+K_3=\rho_1$ and $K_1+K_2+K_3'=\rho_2$. The sum $t+w$ must have the same parity as $l_1+l_2$. Using the properties of the coefficients $\langle K_1K_2K_3|nlm\rangle$ given by Chasman and Wahlborn (1967), the RHS of (21) could be simplified further.

A particularly simple sum rule is obtained from (21) for the case $t=w=0$. This leads to $l=L=0$ and therefore to $\lambda=0$ and $l_1=l_2$. Using the relation $\langle lml-m|00\rangle = (-1)^{l-m}/(2l+1)^{1/2}$ and the orthogonality relation for $\langle K_1K_2K_3|n_1l_1m_1\rangle$, I find the sum rule

$$\sum_{n+N=n_1+n_2+l_1}(-1)^n\left(\frac{4\Gamma(n+\frac{3}{2})\Gamma(N+\frac{3}{2})}{\pi(n!)(N!)}\right)^{1/2}(nlNl0|n_1l_1n_2l_10)\delta_{l0}=\delta_{n_1n_2}(2l_1+1)^{1/2}. \qquad (23)$$

For the special case of $n_1=n_2$, the sum rule in (23) can be written in a different form. Utilising the orthogonality relation for the TBM coefficients and summing over $n_1$ and $l_1$ with the restriction $2n_1+l_1=\rho_1$, I find that

$$\sum_{2n_1+l_1=\rho_1}(2l_1+1)^{1/2}(nlNl0|n_1l_1n_1l_10)=(-1)^n\left(\frac{4\Gamma(n+\frac{3}{2})\Gamma(N+\frac{3}{2})}{\pi(n!)(N!)}\right)^{1/2}\delta_{l0}. \qquad (24)$$

This is the same expression derived earlier by Shlomo and Prakash (1981, see equation (33)).

Sum rules involving the sum over the row and column indices of the TBM coefficients can be obtained by summing over $n_1, l_1, n_2, l_2$ in (20) (or (21)) with the restrictions that $2n_1+l_1=\rho_1$ and $2n_2+l_2=\rho_2$. The resulting sum-rules can be simplified for certain values of $(r, s, t, u, v, w)$, using the orthogonality relations and the explicit expressions for the coefficients appearing in the sum rules. A particulary simple form is found from (21) for the case $(n_1l_1)=(n_2l_2)$. By multiplying (21) by $(-1)^{l_1-m}\langle l_1ml_1-m|\lambda 0\rangle$, using the relation $(-1)^{l_1-m}=(2l_1+1)^{1/2}\langle l_1ml_1-m|00\rangle$, summing over $\lambda$ and $m$, and employing the orthogonality relations for the Clebsch–Gordon coefficients, one finds that the LHS vanishes unless $\lambda=0$. Finally the expression

$$\sum_{2n_1+l_1=\rho_1}\sum_{n+N+l=\rho_1}(-1)^l\left(\frac{2l_1+1}{2l+1}\right)^{1/2}D_{tw}^{nlNl}(nlNl0|n_1l_1n_1l_10)$$
$$=(-1)^{w/2}\binom{\rho_1+2}{(2\rho_1-t-w)/2}\Big/[(\tfrac{1}{2}t)!(\tfrac{1}{2}w)!] \qquad (25)$$

is found by taking the sum over $(n_1l_1)$. The simple expression for the RHS of (25) follows from the orthogonality relation for $\langle K_1K_2K_3|nlm\rangle$ and the results of (9) to (12). The sum over $l$ in (25) is restricted by $t-l$ being even and the RHS is replaced by zero if $t$ is odd.

## 3. Summary

In summary, I have derived a new class of sum rules for the HO brackets given by (15) for the one-dimensional case and by (20), (21) and (25) for the three-dimensional case.

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## Appendix

To derive the sum rules for the TBM coefficients I first utilise (19) for $\psi_{nlm}$ and $\psi_{NLM}$ in the LHS of (20). This leads to

$$\begin{aligned}
&\frac{1}{\pi^{3/2}}\sum_{mM}\sum_{nlNL}\langle lmLM|\lambda\mu\rangle(nlNL\lambda|n_1l_1n_2l_2\lambda)\\
&\qquad\times \mathrm{i}^{2n+l}\sum_{a_iA_i}\langle a_1a_2a_3|nlm\rangle\langle A_1A_2A_3|NLM\rangle\\
&\qquad\times \psi_{a_1}(\sqrt{2}p_x)\psi_{a_2}(\sqrt{2}p_y)\psi_{a_3}(\sqrt{2}p_z)\psi_{A_1}(\sqrt{2}X)\psi_{A_2}(\sqrt{2}Y)\psi_{A_3}(\sqrt{2}Z)\\
&\qquad=\sum_{m_1m_2}\sum_{K_iK_i'}\langle l_1m_1l_2m_2|\lambda\mu\rangle\langle K_1K_2K_3|n_1l_1m_1\rangle\\
&\qquad\times\langle K_1'K_2'K_3'|n_2l_2m_2\rangle f_{K_1K_1'}(X,p_x)f_{K_2K_2'}(Y,p_y)f_{K_3K_3'}(Z,p_z). \qquad\text{(A1)}
\end{aligned}$$

Defining $\rho_1=2n_1+l_1$, $\rho_2=2n_2+l_2$ and $\rho=\rho_1+\rho_2$, the sums on the LHS of (A1) are limited by $m+M=\mu$, $2n+l+2N+L=\rho$, $a_1+a_2+a_3=2n+l$ and $A_1+A_2+A_3=2N+L$. The sums on the RHS of (A1) are limited by $m_1+m_2=\mu$, $K_1+K_2+K_3=\rho_1$ and $K_1'+K_2'+K_3'=\rho_2$. Using (2) and (3) for $\psi_{a_i}$ and $\psi_{A_i}$ in the LHS of (A1) and the expression (11) for $f_{K_iK_i'}$ in the RHS of (A1) and equating the coefficients of $(\mathrm{i}p_x)^r(\mathrm{i}p_y)^s(\mathrm{i}p_z)^tX^uY^vZ^w$ of both sides, one finds the sum rule

$$\begin{aligned}
&\sum_{mM}\sum_{nlNL}\langle lmLM|\lambda\mu\rangle(nlNL\lambda|n_1l_1n_2l_2\lambda)G^{nlmNLM}_{rstuvw}\\
&\qquad=\sum_{m_1m_2}\sum_{K_iK_i'}\langle l_1m_1l_2m_2|\lambda\mu\rangle\langle K_1K_2K_3|n_1l_1m_1\rangle\\
&\qquad\times\langle K_1'K_2'K_3'|n_2l_2m_2\rangle r!\,u!\,C^{K_1K_1'}_{ru}s!\,v!\,C^{K_2K_2'}_{sv}t!\,w!\,C^{K_3K_3'}_{tw}\\
&\qquad\times\langle ru|\tfrac{1}{2}(r+u+K_1-K_1')\tfrac{1}{2}(r+u-K_1+K_1')\rangle\\
&\qquad\times\langle sv|\tfrac{1}{2}(s+v+K_2-K_2')\tfrac{1}{2}(s+v-K_2+K_2')\rangle\\
&\qquad\times\langle tw|\tfrac{1}{2}(t+w+K_3-K_3')\tfrac{1}{2}(t+w-K_3+K_3')\rangle \qquad\text{(A2)}
\end{aligned}$$

for each set of integers $(r, s, t, u, v, w)$ with the restriction $r+s+t+u+v+w\leq\rho$. The $C$-coefficients in (A2) are defined in equation (12) and the $G$'s are given by

$$\begin{aligned}
G^{nlmNLM}_{rstuvw}&=\sum_{a_iA_i}(-1)^{(2N+L-u-v-w)/2}\langle a_1a_2a_3|nlm\rangle\\
&\quad\times\langle A_1A_2A_3|NLM\rangle(2^{-(\rho_1+\rho_2-r-s-t-u-v-w)}a_1!\,a_2!\,a_3!\,A_1!\,A_2!\,A_3!)^{1/2}
\end{aligned}$$

$$\times\left[\left(\frac{a_1-r}{2}\right)!\left(\frac{a_2-s}{2}\right)!\left(\frac{a_3-t}{2}\right)!\left(\frac{A_1-u}{2}\right)!\left(\frac{A_2-v}{2}\right)!\left(\frac{A_3-w}{2}\right)!\right]^{-1}. \quad \text{(A3)}$$

The transformation coefficients $\langle kK|K_1K_2\rangle$ are given in (6) and the explicit expression for the transformation coefficient $\langle K_1K_2K_3|nlm\rangle$ was derived by Chasman and Wahlborn (1967).

It should be emphasised that one obtains a set of sum rules for any given values of $n_1$, $l_1$, $n_2$, $l_2$, $\lambda$ and $\mu$. For the special case in which $r+s+t+u+v+w<|\rho_1-\rho_2|$, the RHS of (A2) vanishes, leading to a particularly simple sum rule. Also, using the properties of the Clebsch–Gordon coefficients and the transformation coefficients $\langle K_1K_2K_3|nlm\rangle$ (see Chasman and Walhborn 1967), simplified forms of the sum rules can be derived for special values of $r$, $s$, $t$, $u$, $v$ and $w$. A specific example is discussed in the text.

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