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Received June 18, 1992

We study the thermodynamic concept of isolation. The causal motion of a system that models a thermodynamic "universe" but nevertheless couples to a surround is reconciled with an increase of entropy—in the manner of the second law of thermodynamics—for the system. The system's ket space is *n*-dimensional, the surround's is K-dimensional, and the initial state is taken "purepure": the tensor product of a pure *n*-state with a pure K-state. Near-maximal entropy is found for the reduced *n*-state in deep time, first for most random Hamiltonians, then also under restriction to weak *n*-K coupling—but then with a shortfall of about 1 bit.

## **1. THE HOMOGENEOUS MEAN TRACE OF THE SQUARE**

Where does entropy come from? The reduced density matrix  $\rho$  of a subsystem is usually mixed, even if the larger, enveloping state is pure. Indeed, near-maximal entropy is found from just this reduction. Here we look at a random enveloping unit vector's state matrix  $uu^{\dagger}$ , bypassing motion, so there is as yet no Hamiltonian. Our so-called HOMOGENEOUS notion of randomness is a distribution uniform in the "area" on the unit sphere. We begin with a newly styled account of Lubkin (1978) as a suitable preface, after further introductory conventions and bows.

Notation. The usual convention of implied summation over twicerepeated indices applies. More complicated sums will be explicit. Lowercase Roman labels  $i, j, \ldots$  run over n distinct values, uppercase Roman labels over K values; Greek labels run over nK values; but early lowercase Roman labels a, b, c, d share some domain of common, unspecified size N.

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Abbreviation. "trsq" for "trace of the square." We consider the mean first over a homogeneously distributed unit vector  $u_{iA}$  in *nK*-dimensional Hilbert space—of the trsq of the reduced density matrix  $\rho$  obtained from the projection on *u*, by tracing over the *K*-labels (our jargon: "Landau" tracing). In symbols: trsq = trace( $\rho^2$ ), where  $\rho_{ij} = u_{iA}u_{iA}^*$ .

In this Section 1 we review (Lubkin, 1978) the homogeneous averaging of *trsq* to "*HMG* $\langle trsq \rangle$ "—or briefly to  $\langle trsq \rangle$  when the sort of averaging is clear—and thereafter we note the link to the second law of thermodynamics, of the resulting identity *HMG* or equation (1).

Two other, newer sorts of averagings, called ISOTROPIC—ISTR, equation (7)—and WEAK—WK, equation (12)—will be developed in later sections. They will yield progressively finer links between (quantum) mechanics and the second law of thermodynamics, the WEAK being perhaps reminiscent of Boltzmann's H-theorem in its intent.

On, then, to resume development of the HOMOGENEOUS average. The result, (1) or *HMG*, is given in terms of *trsq*, rather than in terms of the less symmetric *impurity* = (1 - trsq)/(1 - 1/n) of Lubkin (1978); it is

$$\langle trsq \rangle = \frac{n+K}{nK+1}$$
 HMG (1)

Derivation of *HMG*, equation (1):  $\langle trsq \rangle$  is  $u_{iA}u_{jA}^*$  squared, traced, and averaged:

$$\langle trsq \rangle = \langle u_{iA} u_{jA}^* u_{jB} u_{iB}^* \rangle \qquad preQRTC \quad (2)$$

Go to rules for means of products of Cartesian components: Product of Kronecker deltas 1, times a numeric, deltas only between conjugates,  $\dots$ . Our quartic pattern in equation (2), namely

$$\langle ab^*cd^* \rangle$$
, yields  $C(1_{ab}1_{cd}+1_{ad}1_{bc})$ 

Fix constant C through an inductive stepdown:

Vector u is a unit vector, so  $\langle u_a u_a^* \rangle = \langle 1 \rangle = 1$ . On the other hand, the quadratic analog of the quartic pattern evaluates

$$\langle u_a u_b^* \rangle = C' \mathbf{1}_{ab}$$

for some other unknown constant C'. Let N be the dimension (which is nK for our first application). Contraction gives  $\langle u_a u_a^* \rangle = C'N$ , whose known value 1 gives C' = 1/N. Hence

$$\langle u_a u_b^* \rangle = \frac{1}{N} \mathbf{1}_{ab}$$

is the length-2 QUADRATIC "answer"; abbreviated

$$\langle ab^* \rangle = \frac{1}{N} \mathbf{1}_{ab}$$
 QDRT (3)

Use QDRT, equation (3), to now find the quartic pattern's C by a contraction:  $\langle ab^*cc^*\rangle = \langle ab^*\rangle = (1/N)1_{ab}$  also equals  $C(1_{ab}1_{cc}+1_{ac}1_{bc})$ , which is  $C(1_{ab}N+1_{ab}) = C(N+1)1_{ab}$ . Hence C = 1/N(N+1), which completes our length-4 answer:

$$\langle ab^*cd^* \rangle = \frac{1}{N(N+1)} (1_{ab} 1_{cd} + 1_{ad} 1_{bc}) \qquad QRTC \quad (4)$$

Apply QRTC, equation (4). The overall dimension is now N = nK, and

$$\langle u_{iA} u_{jA}^* u_{jB} u_{iB}^* \rangle = \frac{1}{nK(nK+1)} \left( 1_{iAjA} 1_{jBiB} + 1_{iAiB} 1_{jAjB} \right)$$
$$= \frac{1}{nK(nK+1)} \left( 1_{ij}K 1_{ji}K + n 1_{AB} n 1_{AB} \right)$$
$$= \frac{1}{nK(nK+1)} \left( nK^2 + Kn^2 \right)$$

from which nK cancels to give HMG, equation (1).

### Discussion

*HMG*, equation (1), already goes far to finger the normalized unit matrix as a good approximation to a typical reduced density matrix when K is large: The limit of the  $\langle trsq \rangle$  value (n+K)/(nK+1) as K goes infinite is evidently 1/n. This is also the trsq of the trace-normalized n-dimensional unit matrix. As all other n by n density matrices have larger trsq, closeness in regard to this single statistic trsq suffices to establish closeness matricially to the normalized unit matrix.

Import? Landau tracing not only generates entropy in an *n*-sector of interest, but generates *enough* entropy to support the second law of thermodynamics.

On the other hand, maximal entropy, when K < n, is only ln K, so the normalized unit matrix, of larger entropy ln n, cannot even occur as a reduced density matrix, unless  $K \ge n$ . Let the case K = n then be our notion of *small surround*. Here (n + K)/(nK + 1) reduces to  $2n/(n^2 + 1)$ , which is roughly 1/(n/2). That is the *trsq* value for a trace-normalized unit matrix in half the system's dimension, which shrunken matrix has entropy 1 bit less than the *n*-dimensional normalized unit matrix. So the penalty for a "small surround" appears to be about a 1-bit shortfall in the entropy from the maximum possible value ln n favored by the second law.

We shall see a 1-bit shortfall appear later, for a different reason, when we consider instead the interaction of an *n*-system with the more usual large-K surround  $(K \gg n)$  when we impose the restriction that interaction with the surround be WEAK.

### 2. EHRENFESTS

This whole business, beyond HMG, equation (1), stems from a quantal improvement (Lubkin and Lubkin, 1990) on the Ehrenfests' urn model (Klein, 1970).

Start with a "purepure" state—tensor product of pure *n*-state with pure K-state—but let a time-independent Hamiltonian H move it. Overall purity will of course be maintained, but *purepurity* will [almost always] be lost; curves showing that loss, e.g., graphs of *trsq* falling from value 1 at time t = 0, then oscillating, carry the same intuitive sense as the Ehrenfests' aleatory model: development of a fluctuating entropy, etc.—while yet eschewing anything aleatory in the process of evolution in time. Perhaps needless to say, the arbitrariness of the sort of H we favor, a matrix chosen randomly, does inject an aleatory quality, but no "dice" get thrown as time passes.

We have a random law of motion, not a law of random motion!

### **3. DEEP TIME**

Does  $\langle trsq \rangle$ , but now averaged over time, still evaluate to HMG, equation (1)?

Of course not: The result depends on choices, which H and which initial purepure state. More geometrically: The motion, while [almost always] ergodic over the *nK*-real-dimensional motional torus marked by *nK* increasing phases of the Hamiltonian's *nK* eigenkets, does not go everywhere, because that torus is a *proper* submanifold of the whole sphere of *nK*-complex-dimensional unit vectors.

But is answer *HMG*, (1), recovered when time-averaged *trsq*'s are *further* averaged ISOTROPICALLY over *H*'s? We make this "isotropy" of Hamiltonians precise, and find "almost, but not quite": our initial purepurity does bias the isotropic average  $\langle trsq \rangle$  a small amount  $\Delta$  above *HMG*.

To reach  $\Delta$ , equation (7), and also to enable fetching a time-meaned *trsq* without approximating from an actual Monte Carlo run, we first get DEEPTIME formula *DPT*, (6), where *H* and the initial state are fixed. [Monte Carlo runs indeed check *DPT*, equation (6).] This story is here abbreviated to making precise our "isotropic" distribution of *H*'s, then giving "an early suggestive step," and then one version of the result—*DPT*, (6) [which we repackaged, however, for faster computation].

"Isotropic" Defined. N by N Hermitian matrices A, B, ... form a vector space under real linear combination. With real inner product "trace AB," these Hermitians form a real Euclidean  $N^2$ -dimensional metric space. It is

when we think of Hamiltonians as real vectors in this Euclidean sense that we simply ask for an isotropic distribution. To attain this isotropy on a computer, we select Cartesian components subject to a Gaussian random process: easy. [We are not presenting outputs here; but these were important in keeping us honest and confident in going from one step to the next! See Lubkin and Lubkin (1990) for a few outputs.]

"An Early Suggestive Step," equation (5), is obtained from equation (2) by expanding an initial ket  $|y\rangle$  on the Hamiltonian's eigenbasis. This step,

$$trsq(t) = (iA|\alpha\rangle\langle\beta|jA)(jB|\gamma\rangle\langle\delta|iB) \exp[\sqrt{-1}(E_{\beta} - E_{\alpha} + E_{\delta} - E_{\gamma}) \times t] \times \langle\alpha|y\rangle(y|\beta\rangle\langle\gamma|y\rangle(y|\delta\rangle)$$
(5)

features nK Greek-labeled angular-bracketed kets  $|\cdot\rangle$  eigen for the Hamiltonian, but also round-bracketed kets  $|\cdot\rangle$  which constitute what we call our "spindle" basis,  $|iA\rangle$  being the *i*th basic *n*-space vector tensor-multiplied into the Ath basic K-space vector. Thus  $|\cdot\rangle$  defines our notion of the *nK*-space as "constituted of an *n*-part and a K-part."

Rejecting a population of zero measure allows us to pass to the generic case, where the exponential in time t mostly averages to 0; otherwise to 1, and 1 precisely when  $\beta$  is either  $\alpha$  or  $\gamma$ , and the other two Greek indices also match.

The result is DEEPTIME formula DPT, (6):

$$DPT trsq = -\sum_{\alpha} (iA|\alpha\rangle\langle\alpha|y)(y|\alpha\rangle\langle\alpha|jA)(jB|\alpha\rangle\langle\alpha|y)(y|\alpha\rangle\langle\alpha|iB)$$
$$+\sum_{\alpha} (iA|\alpha\rangle\langle\alpha|y)(y|\alpha\rangle\langle\alpha|jA) \sum_{\gamma} (jB|\gamma\rangle\langle\gamma|y)(y|\gamma\rangle\langle\gamma|iB)$$
$$+\sum_{\alpha} (iA|\alpha\rangle\langle\alpha|y)(y|\alpha\rangle\langle\alpha|iB) \sum_{\beta} (jB|\beta\rangle\langle\beta|y)(y|\beta\rangle\langle\beta|jA)$$
$$DPT \quad (6)$$

[In runs, without loss of generality under our desideratum of purepure factorizability of initial ket  $|y\rangle$ , we used a single basic spindle ket for  $|y\rangle$ ; in symbols,  $|y\rangle = |i_0A_0\rangle$ .]

*Remarks.* Only "direction cosines" between spindle  $|\cdot\rangle$  and eigenbasis  $|\cdot\rangle$  occur in *DPT*, (6). So further ISOTROPIC averaging of (6) is pure geometry, hence clean fun, and perhaps this is why we did it. The products are all of eight such cosines, and that forced us to parallel the earlier identities *QDR*, (3), and *QRT*, (4), with an *octic* identity featuring two vectors rather than just one—as the main tool along the way. That lengthy computation is omitted, but the answer is as follows:

The ISOTROPIC average (7) of the deeptime average DPT (6) of trsq is given by

$$HMG\langle trsq \rangle = \frac{n+K}{nK+1}$$

$$ISTR\langle trsq \rangle = HMG\langle trsq \rangle + \Delta \qquad ISTR \quad (7)$$

$$\Delta = \frac{2(nK+1-n-K)}{nK(nK+1)(nK+3)}$$

The increment  $\Delta$  is indeed small compared to the old part (1), *HMG*, of the answer—(7) or *ISTR*. Even in the 2, 2 case (n = 2 and K = 2), where *HMG* is  $\frac{4}{5} = \frac{56}{70}$ ,  $\Delta$  is already only  $\frac{1}{70}$ .

The attainment of near-maximal entropy through encompassing mechanical motion from a start at zero entropy, in the typical case favored by an ISOTROPICally distributed choice of Hamiltonian, is now established, by this smallness of  $\Delta$ . The limit of ISTR, (7), as K goes infinite remains 1/n. The value of ISTR  $\langle trsq \rangle$ , equation (7), for the case K = n of small surround exceeds the corresponding equation (1), HMG, value,  $2n/(n^2+1)$ , by only  $2(n^2-2n+1)/[n^2(n^2+1)(n^2+3)]$ , so that even for small surround, ISTR  $\langle trsq \rangle$ , like HMG  $\langle trsq \rangle$ , is still near 1/(n/2), and the estimate of 1-bit shortfall in the entropy from smallness of the surround stands as before.

### 4. WEAK INTERACTION

But all is not yet well. The mean looks at nK by nK Hamiltonians so isotropically as to make no distinction between *n*-system, *K*-system, and their coupling. If both systems are so thoroughly tied together, then perhaps it is not reasonable to treat them separately at all. Most transparently, strong coupling is surely inconsistent with thermodynamic *isolation* of the *n*system.

So we look instead, now, at Hamiltonians

$$H = H$$
sys +  $H$ sur +  $H$ int

that are each a sum of an *n*-part for the system,  $H_{\text{sys}_{iAjB}} = h_{\text{sys}_{ij}} 1_{AB}$ , of a *K*-part for the surround,  $H_{\text{sur}_{iAjB}} = 1_{ij}H_{\text{SUR}_{AB}}$ , and of a still generic interaction part Hint, made weak, however, by being multiplied by a small positive parameter  $\lambda$ . [What we did on the computer was to first ISO-TROPICally pick a random generic precursor  $H_{iAjB}$ , Gaussianly as before, from which the parts *h*sys and *H*SUR were picked out, by the two appropriate partial (Landau) tracings; we could also scale *h*sys and *H*SUR by respective parameters  $\mu$  and  $\nu$ . The residue, now trace-orthogonal to both forms "matrix<sub>ij</sub>  $1_{AB}$ " and " $1_{ij}MATRIX_{AB}$ ," was scaled by  $\lambda$  to give Hint.]

The "weak limit" then imposes

$$\lambda \ll \mu, \qquad \lambda \ll \nu \qquad DEF WEAK$$
(8)

Does this WEAK bias away from ISOTROPICity spoil the attainment in the mean of the minimal *trsq* value 1/n in the limit of large K? Indeed the second law *is* challenged, but "only a bit": The weak limit of *trsq*, with also K put infinite, gets enlarged to 1/[(n+1)/2], near enough to 1/(n/2) to indicate an entropic shortfall of about 1 bit. The following sketches the way to the WEAK results—*WK DPT*, equation (9), for a generic weak run—and *WK*, equation (12), the isotropized of (9), for *trsq*.

All we need is to apply DPT, equation (6), once more. That was good for any generic Hamiltonian, that is, any  $|H_{iAjB}|$  whose nK eigenvalues are linearly independent over the rationals. Fooling around with  $\lambda$ ,  $\mu$ , and  $\nu$ , all positive, does not spoil the measure-zero quality of rational dependence; hence DPT, equation (6), will still apply to almost all runs, hence to getting a new WEAKly meaned *trsq*. We must choose  $\lambda$  small, but not zero, and look at runs deep in time, which is, formally, to take the limit of infinite time first, before putting  $\lambda$  to zero. Conveniently, this is automatically accomplished by simply using unweak formula DPT, (6), before specializing to weak. In the weak limit, the nK-eigenkets  $|\alpha\rangle$ , etc., tensor-factor into *n*-eigenkets of hsys and K-eigenkets of HSUR; thus,  $|\alpha\rangle = |iA\rangle = |i\rangle|A\rangle$ . A typical "direction cosine"  $(jB|\alpha\rangle$ , say, in equation (6), would now become (jB|iA), which factors into  $(j|i\rangle(B|A)$ . Skipping over some algebra, we give the surprisingly compact result for a generic weak run:

$$\langle trsq \rangle = x + y - xy$$
 WK DPT (9)

where

$$x = \sum_{i} |(i_0|i)|^4 \qquad DEFx \quad (10)$$

is the sum of fourth powers of the absolute value of the inner product between the initial *n*-ket and the direction of each *n*-space eigenket; and where y is the analogous quantity for the K-space:

$$y = \sum_{A} |(A_0|A)|^4 \qquad DEFy \quad (11)$$

Here the brackets  $\langle \cdot \rangle$  around *trsq* signify averaging in time, over a run, and we have yet to average also over weak Hamiltonians, that is to say, ISOTROPICally, but subject to the imposition of coefficients  $\lambda$ ,  $\mu$ ,  $\nu$ , with  $\lambda$  small.

But  $\lambda$ ,  $\mu$ ,  $\nu$  already do not survive in formulas (10) and (11). So all that remains to effect the ISOTROPIC WEAK averaging is to average x + y - xy. Here x depends only on the way the initial *n*-ket splits on the

*n*-eigenframe, y only on how the initial K-ket splits on the K-eigenframe, and all is once more simply geometry, indeed with n and K separated.

To get an ISOTROPIC WEAK average  $\langle x \rangle$  in place of x, we resort again to QRT identity (4), namely

$$\langle ab^*cd^* \rangle = \frac{1}{N(N+1)} (1_{ab} 1_{cd} + 1_{ad} 1_{bc})$$

but now with a = b = c = d and N = n, to get the mean for a single component's fourth power, namely  $\langle aa^*aa^* \rangle = 2/n(n+1)$  for each fixed value of a. Summing on a then yields

$$\langle x \rangle = \frac{2}{n+1}$$

Similarly,

$$\langle y \rangle = \frac{2}{K+1}$$

and

$$ISTR \ WK\langle trsq \rangle = \langle x \rangle + \langle y \rangle - \langle x \rangle \langle y \rangle$$
$$= \frac{2}{n+1} + \frac{2}{K+1} - \frac{4}{(n+1)(K+1)}$$
$$ISTR \ WK\langle trsq \rangle = \frac{2(K+n)}{(K+1)(n+1)} \qquad WK \quad (12)$$

The limit for large K is 2/(n+1), about twice the unweak minimum *trsq* of 1/n, thus indicating an entropic shortfall of about 1 bit, to slightly weaken our confidence in mechanical support for the second law! If we instead put K = n (*small surround*), we find  $4n/(n+1)^2$ , a shortfall of about 2 bits: showing that the weak- and small-surround shortfalls are different matters, by refusing to fuse here.

Approach to weak interactions by PARADOXES [and REFUTA-TIONS]:

- In the infinitely weak limit, purepurity is preserved, hence isotropic weak *trsq* should be 1, and not WK, (12), as stated! [Wrong order of limits of weakness zero and time infinite.]
- So avoid this mistake by a finite but very weak interaction. Still keep purepurity, because each exact energy is near one unperturbed energy; hence NO amount of waiting will give transitions!

[Truly there are negligibly few transitions; indeed, this is the traditional isolation of the second law! The mistake is in tacitly addressing the single energy level. A free purepure state begins expanded over many levels.]

• But that superposition will not help, because purepurity initially demands a product of an *n*-superposition with a *K*-superposition, and nothing more complicated. The *n*-one does its motion, the *K*-one its, hence the factorization remains unspoilt, and the right answer remains 1!

[This merely reverts to not giving the weak interaction enough time. Indeed, the generic weak interaction adds a different small random energy to each of the nK eigenvalues—in first-order perturbation theory the expectation value of the interaction Hamiltonian—to the unperturbed n- and K-energies. In time, these nK different small increments generate large phase angles. The initial phasing that effects factorization—purepurity—is thereby ruined.]

Detail. We observed in actual runs that large nK goes with random Hamiltonians that *individually* demonstrate average behavior. This is reasonable, in retrospect: Indeed, arbitrarily split the set of eigenspaces of the reduced density matrix into subsets. Owing to the arbitrariness, the same statistical facts will hold in each subset. Statistics of all the eigenvalues together would then be seen as averaging over similar subpopulations, hence subject to a law of large numbers, and so to a conformity between the typical and the average.

This "detail" partly refutes the objection that this work is empty of physical content, in refusing to focus on any particular Hamiltonian, by fancifully choosing to average our statistic (trsq) over (infinitely) many Hamiltonians. "Partly": ISOTROPIC bias indeed acts in our *nK* Gaussian choices of matrix element, in upping even a single Hamiltonian.

# 5. THERMODYNAMIC ISOLATION

This perhaps repeats our second paradox-and-refutation, but it is worth the space, as the mystery of thermodynamic isolation is the whole point of this work. Mystery? A mechanically isolated system, by definition, moves under Schrödinger's Hamiltonian-driven equation, hence maintains the eigenvalues of its density matrix; in particular, its entropy is conserved. But the second law of thermodynamics would have the entropy of an *isolated* system increase to a maximum. This conflict forces us to regard *thermodynamic* isolation as being distinct from *mechanical*. A thermodynamically isolated system must be coupled to a surround strongly enough to damage purepurity, in the manner of our WEAK interaction, while yet sharing some quality in common with the more rigorous mechanical sort of isolation. So our model of the thermodynamic system is the *n*-dimensional ket space, coupled WEAKly to a K-dimensional ket-space surround. Entropic isolation is spoilt, for the benefit of the second law, but then what "isolation" is left? We still have conservation of the *n*-system's own energy, in a detailed manner, and not just in the sense of balance against the K-system acting as a heat bath. The "reservoir" in the title of Lubkin (1978), while appropriate for less-weak coupling, has here become "surround," precisely to avoid the implication that it is a heat bath, in the present context of weak limit. Indeed, the *n*-system is here the model for a complete thermodynamic UNIVERSE, including all baths. The only function served by the K-system is the disordering of the *n*-system, to satisfy the second law's demand for disorder—of a thermodynamically isolated entity, or "universe."

Hence the *n*-system must have a reasonably strict conservation of its own energy, in spite of its weak coupling to the K-system. This conservation of *n*-energy is what we do in fact get from first-order time-independent perturbation theory: The perturbed energies are of course conserved, but also each perturbed energy lies close to one unperturbed sum of an *n*-energy and a K-energy—where we neglect degeneracies as accidents of no measure. Thus, weakness does preserve the *n*-energy.

This conclusion does not reach our goal, of understanding increase of the *n*-entropy, if we restrict it to a single energetic eigenstate, for then purepurity will never get markedly broken, and *n*-entropy will not markedly increase. We must rather contemplate a general state. The probabilities of distinct *n*-energies are preserved; and this is the thermodynamic isolation we seek: "unobserved energetic microcanonicality." Entropy of the *n*-system grows to near maximum, hence—incidentally—cannot coincide with the essentially constant formal entropy,  $-\sum p \ln p$ , cooked up from the energetic probabilities *p*, which vary negligibly in time. Indeed, the *n*-system's reduced density matrix  $\rho$  does *not* start out codiagonal with the *n*-energy.

There is also no further *n*-conservation, aside from conservation of energy, within this model: Other conserved quantities would render the energy degenerate, and our random Hamiltonians almost always avoid that.

### ACKNOWLEDGMENT

We thank Ming Lap Chow for telling us about the closeness of our work to "decoherence," and in particular to a preprint of Andreas Albrecht, confirmed by a talk here of Albrecht's. For instance, we both adopted the same word *weak* for the same notion, independently, with reckless disregard for the beta-decay sense of "weak"! The models may differ slightly, owing to our Gaussian grasp on isotropicity.

### NOTE ADDED IN PROOF

Don N. Page has kindly sent us a manuscript wherein he confirms and sharpens the Lubkin (1978) estimate of the small deficit in *n*-system's entropy within an enveloping random pure nK state.

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