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Representative state in incomplete quantal state determination

I D Ivanović

Department of Physics, Faculty of Sciences, POB 550, 11 000 Belgrade, Yugoslavia

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Abstract. The choice of a representative state in an incomplete quantal state determination is reconsidered and two main possibilities, the most probable and the expected representative state are compared. It is shown that probability densities over a set of states, underlying an expected state, are in complete agreement with the standard quantal formalism. Examples for some simple densities are given and discussed.

1. Introduction

In this paper we will reconsider the choice of a representative state (RS) in an incomplete state determination (SD). This problem has been discussed by Jaynes (1957), Wichmann (1963) and by Park and Band (1976). We will adopt the point of view proposed by the last authors. However, the projection postulate (von Neumann 1955) will be explicitly used throughout and the result will be a more formal, geometrised description of a SD.

A brief exposition of the problem may be the following one. The choice of a Rs has two parts. The first one is to obtain, from the results of different quantal measurements, a set of admissible states for the inspected ensemble which is described by a fixed but unknown state. The second part based on some further assumptions about the state of the inspected ensemble should result in the very choice of a Rs out of the set of admissible ones. The essential assumption is that the inspected ensemble is available in a large number of replicas which should be subjected to different measurements. A Rs will describe a replica which has not been inspected by an observer.

The paper is organised as follows. In § 2 we will give a brief description of the set of states, measurements and SD in a finite-dimensional case. Section 3 contains an analysis of the standard, maximum entropy RS which is followed by the definition of an 'expected' RS proposed by Park and Band (1976) and Band and Park (1976). In § 4 we will give some simple relations between 'expected' states and their standard quantal counterparts. In § 5 four examples of probability densities, underlying any expected state, will be inspected.

2. States and their description

In this section we will reconsider the set of states in a finite-dimensional case (cf Harriman 1978, Ivanović 1981).

To every collection of quantal systems, one can assign a state \hat{W} , $\hat{W} \ge 0$, $Tr(\hat{W}) = 1$, which will describe all relevant properties of the collection mentioned.

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It is useful to think of these states as elements of the real vector space of Hermitian operators acting on the Hilbert space H attached to the inspected ensemble. This real vector space will be denoted by $V_h = \{\hat{A} | \hat{A}^+ = \hat{A}\}$. Introducing the scalar product as $(\hat{A}, \hat{B}) \equiv \text{Tr}(\hat{A}\hat{B})$ and norm $\|\hat{A}\| = (\text{Tr}(\hat{A}^2))^{1/2}$, V_h becomes an n^2 -dimensional real Euclidian space, where n is the dimensionality of the underlying vector space H.

The set of all states $V_w = \{ \hat{W} | \hat{W} \ge 0, \operatorname{Tr}(\hat{W}) = 1 \}$ is a convex set in V_h . Its extremal points are pure states, $\hat{W}^2 = \hat{W}$, i.e. they are one-dimensional projectors; we will denote them by a properly indexed \hat{P} .

A non-degenerate observable $\hat{A} = \sum_k a_k \hat{P}_k$ will induce an orthonormalised basis in V_h ;

$$\hat{P}_{k}, \quad 1 \leq k \leq n, \qquad \hat{\sigma}_{mk}^{(r)} = (2)^{-1/2} (\hat{e}_{km} + \hat{e}_{mk}),
\sigma_{mk}^{(i)} = i(2)^{-1/2} (\hat{e}_{km} - \hat{e}_{mk}), \qquad 1 \leq k < m \leq n$$
(1)

where matrix elements of \hat{e}_{mk} are $[\hat{e}_{mk}]_{rs} = \delta_{mr}\delta_{ks}$ in the basis in which $\hat{P}_k = \hat{e}_{kk}$. In particular, by $V_h(\{\hat{P}_k\})$ we will denote the *n*-dimensional subspace of mutually commuting operators. Furthermore $V_W(\{\hat{P}_k\}) = V_w \cap V_h(\{\hat{P}_k\})$ will be the convex set of mutually commuting states, coinciding with a regular *n*-dimensional simplex.

If an ensemble is described by a state \hat{W} in the measurement of a non-degenerate observable $\hat{A} = \sum_k a_k \hat{P}_k$ the state \hat{W} will suffer the change (von Neumann 1955)

$$\hat{W} \rightarrow \hat{W}' = \sum_{k} \hat{P}_{k} \hat{W} \hat{P}_{k} \in V_{W}(\{\hat{P}_{k}\}).$$
⁽²⁾

In V_n equation (2) is the orthogonal projection of \hat{W} into $V_n(\{\hat{P}_k\})$ and this projection \hat{W}' lies in $V_W(\{\hat{P}_k\})$.

On the other hand, a state determination (SD) is an attempt to assign a state to an ensemble of quantal systems from the results of different quantal measurements. We will assume that all measurements are in accordance with (2). When a SD results in a single state it is a complete SD, otherwise it is an incomplete SD. Generally a SD procedure composed out of N measurements, e.g. corresponding to the observables $\{\hat{A}^{(s)} = \sum_k a_k^{(s)} \hat{P}_k^{(s)}\} \le s \le N$ will result in a complete SD only if $\{\hat{P}_k^{(s)}\} \le k \le n; 1 \le s \le N$ contains a basis for V_h . Then $\{\hat{A}^{(s)}\}$ is a quorum in V_h (Park and Band 1971).

A simple case of an incomplete SD may occur when the result of a single measurement is a mixed state $(\hat{W}^2 \neq \hat{W})$ and when this result is used for a SD. Let this state be $\hat{W}^{(1)} = \sum_k \hat{P}_k^{(1)} \hat{W}_u \hat{P}_k^{(1)}$ so that $\hat{W}^{(1)} = \sum_k w_k \hat{P}_k^{(1)}$ the projection of \hat{W}_u into $V_W(\{\hat{P}_k\})$ is the only result one has. The only conclusion is that $\hat{W}_u \in V_W(\hat{W}^{(1)}) =$ $\{W|\sum_k \hat{P}_k^{(1)} \hat{W} \hat{P}_k^{(1)} = \hat{W}^{(1)}\}$. The convex set $V_W(\hat{W}^{(1)})$ will be called the set of admissible states for $W^{(1)}$. After k measurements the corresponding set of admissible states will 'shrink' into $W_W(\hat{W}^{(1)}, \ldots, \hat{W}^{(k)}) = \bigcap_r V(\hat{W}^{(r)})$. In the rest of this paper a set of admissible states will be denoted by V_W^{ad} when a particular specification is not necessary. Such sets are always convex, they may have a lattice structure in the sense of the order relation '>' (cf Wehrl 1978) etc.

Sometimes a need for a representative state (RS) $\hat{W}_{RS} \in V_w^{ad}$ may occur. Due to the fact that V_w^{ad} exhausts all objective (measurement based) information concerning the unknown state \hat{W}_u , some further assumptions are necessary in order to obtain a reasonable RS.

3. Representative state

In this section we will start with the standard representative state (RS) (Jaynes 1957, Wichmann 1963).

The standard, maximum entropy RS, $\hat{W}_{RS} \in V_W^{ad}$ is

$$\hat{W}_{\rm RS}: S(\hat{W}_{\rm RS}) > S(\hat{W}) \quad \forall \, \hat{W} \in V_W^{\rm ad}$$
(3)

where $S(\hat{W}) = -\sum_k w_k \ln(w_k)$ is the entropy of $\hat{W} = \sum_k w_k \hat{P}_k$. The assumptions underlying RS from (3) may be the following ones.

(1) All elementary events concerning a single measurement e.g. \hat{P}_k are equally probable, $w(\hat{P}_k) = (1/n)$.

(2) A sequence of \hat{N} events $\hat{P}_{i_1}, \ldots, \hat{P}_{i_N}$ (N is a finite but very large number) where $(N_i/N) \sim w_i$ is the relative frequency of \hat{P}_i , will occur with probability p such that

 $\ln(p) \sim (1/N)S(w_1, \ldots, w_n) + \text{constant.}$

Assumptions (1) and (2) are only one of the ways to obtain the main assumption.

(3) The RS is the most probable state assuming the density $\rho(\hat{W}) \sim S(\hat{W})$ to be valid over V_{W}^{ad} .

The first important task is to justify the existence of probability distributions and densities over V_w . Fortunately this follows from the fact that V_h is an Euclidian space allowing the lebesgue measure $dv = dx_1 dx_2 \dots dx_k$, $k \le n^2$ to be introduced in its k-dimensional subspace or a flat. Under these assumptions one may understand V_w as a classical sample space of the appropriate probability space in which elementary event is a point in V_w i.e. a state.

The second important task is then simple, namely one may assume the existence of some $\rho(\hat{W})$ satisfying $\rho(\hat{W}) \ge 0$, $\int \rho(\hat{W}) dv = 1$ and one may define the expected state as

$$\hat{W}^{\rm E} = \int \hat{W} \rho(\hat{W}) \, \mathrm{d}v$$

being a continuous convex combination of $\hat{W} \in V_W$ (clearly, $\hat{W} = \sum_k w_k \hat{P}_k = \sum_k \int w_k \delta(\hat{W} - \hat{P}_k) \hat{W} dv$).

In this paper we will adopt and inspect the proposal of Park and Band that a RS may be chosen as the expected state under the assumed $\rho(\hat{W})$ for $\hat{W} \in V_w^{ad}$ as

$$\hat{W}_{RS}^{E} = \int_{V_{w}^{ad}} \hat{W} \rho(\hat{W}) \,\mathrm{d}v \tag{4}$$

where dv in (4) is the elementary volume in a properly chosen flat in V_h . For example V_W has zero volume in V_h and one must calculate it in the hyperplane $h(\hat{a}|\text{Tr}(\hat{A}) = 1)$ where V_w is an $(n^2 - 1)$ -dimensional convex body, etc.

The choice of $\rho(\hat{W})$ may follow from quite different assumptions and in fact it will be tested by a SD procedure. Some initial $\rho(\hat{W})$, after obtaining some V_{W}^{ad} from measurements, will change into the new density

$$\rho'(\hat{W}) = \rho(\hat{W}) \left/ \left(\int_{V_w^{ad}} \rho(\hat{W}) \,\mathrm{d}v \right).$$
(5)

We will conclude this section by noting that the difference between (3) and (4) is almost identical to the difference between the corresponding concepts for a classical stochastic variable. Therefore, one's choice between the most probable Rs (e.g. equation (3)) and an expected state (equation (4)) will probably depend on the number of systems in a replica of the inspected ensemble and on the stability of the measurement results.

4. Densities and standard quantal formalism

In this section we will reconsider some general aspects of the assumed densities over V_w and their relationship to the standard quantal description.

To start with, we will choose a basis in V_h such as that in equation (1). Then, any $\hat{W} \in V_W$ may be expressed as

$$\hat{W}(\alpha_1,\ldots,\alpha_n^2) = \sum_k \alpha_k \hat{P}_k + \sum_k \alpha_k \hat{\sigma}_k^{(r)} + \sum_k \alpha_k \hat{\sigma}_k^{(1)}$$

where

$$\hat{\sigma}_{12}^{(r)} = \hat{\sigma}_{k=n+1}^{(r)}, \, \hat{\sigma}_{13}^{(r)} = \hat{\sigma}_{n+2}^{(r)}, \dots, \, \hat{\sigma}_{12}^{(i)} = \hat{\sigma}_{n(n+1)/2+1}^{(i)}, \dots, \, \hat{\sigma}_{n-1,n}^{(i)} = \hat{\sigma}_{n^2}^{(i)}.$$

Furthermore let a density, given in the same basis be $\rho(\alpha_1, \ldots, \alpha_{n^2})$ so that

$$\hat{W}_{RS}^{E} = \int_{V_{W}} \hat{W}(\alpha)\rho(\alpha) \, \mathrm{d}v = \sum_{k=1}^{n} \langle \alpha_{k} \rangle \hat{P}_{k} + \sum_{k=n+1}^{n(n+1)/2} \langle \alpha_{k} \rangle \hat{\sigma}_{k}^{(r)} + \sum_{k=n(n+1)/2+1}^{n^{2}} \langle \alpha_{k} \rangle \sigma_{k}^{(i)} \tag{6}$$

where $\langle \alpha_k \rangle = \int \alpha_k \rho(\alpha) \, \mathrm{d}v$.

Calculation of $\langle \alpha_k \rangle$ may be extremely difficult, however, if one is able to calculate $\langle \alpha_k \rangle$, relations with the standard quantal notions will be almost trivial.

The first question may be: how $\rho(\hat{W})$ affects a single measurement e.g. that of $\hat{A} = \sum_k a_k \hat{P}_k$. The first part of the answer will be to calculate the marginal density over $V_W(\{\hat{P}_k\})$ defined by the chosen observable \hat{A} as

$$\mu(\alpha_1,\ldots,\alpha_n)=\int \rho(\alpha_1,\ldots,\alpha_n)\,\mathrm{d}\alpha_{n+1}\,\mathrm{d}\alpha_{n+2}\ldots\,\mathrm{d}\alpha_n^2.$$

This allows one to determine the expected state for a single measurement procedure as

$$\hat{W}_{M}^{E} = \int \hat{W}(\alpha_{1}, \ldots, \alpha_{n}) \mu(\alpha_{1}, \ldots, \alpha_{n}) \, d\alpha_{1} \, d\alpha_{2} \ldots d\alpha_{n} = \Sigma_{k} \langle \alpha_{k} \rangle \hat{P}_{k}.$$
(7)

A simple consequence of (6) and (7) is that $\hat{W}_{M}^{E} = \sum_{k} \hat{P}_{k} \hat{W}_{RS}^{E} \hat{P}_{k}$ where both states, \hat{W}_{M}^{E} and \hat{W}_{RS}^{E} are obtained from the same density. Obviously, this is an indirect way of saying that for an observable, let it again be $\hat{A} = \sum_{k} a_{k} \hat{P}_{k}$

$$\langle \hat{A} \rangle_{\rho(\hat{W})} = \int \rho(\alpha) \operatorname{Tr}(\hat{A}\hat{W}(\alpha)) \,\mathrm{d}v = \operatorname{Tr}(\hat{W}_{\mathrm{RS}}^{\mathrm{E}}\hat{A}) = \operatorname{Tr}(\hat{W}_{\mathrm{M}}^{\mathrm{E}}\hat{A})$$

Indeed, $\operatorname{Tr}(AW(\alpha)) = \sum_{k=1}^{n} a_k \alpha_k$ hence $\int \rho(\alpha) \operatorname{Tr}(\hat{A}\hat{W}(\alpha)) dv = \sum_{k=1}^{n} a_k \langle \alpha_k \rangle$. Clearly it may happen that $\rho(\alpha_1, \ldots, \alpha_n, 0, \ldots, 0) \equiv 0$ i.e. $\rho(\hat{W}) \equiv 0 \forall \hat{W} \in V_W(\{\hat{P}_k\})$ still $\mu(\alpha_1, \ldots, \alpha_n)$ will be a proper density satisfying $\int \mu(\alpha) d\alpha_1 d\alpha_2 \ldots d\alpha_n = 1$ (in these equations $\alpha_n = 1 - \alpha_1 - \ldots - \alpha_{(n-1)}$).

Furthermore the choice of a particular basis in V_h , unitary equivalent to basis (1) should be unimportant due to the fact that $dv = d\alpha_1 \dots d\alpha_n^2$ is invariant under all rotations in V_h , a fortiori for those which correspond to the unitary transformations over H, i.e. when $A' = UAU^+$.

We will conclude this section with a few remarks concerning the choice of an initial 'complete ignorance' density. There are at least two proposals: $\rho(\hat{W}) \sim S(\hat{W})$ underlying equation (3) and $\rho(\hat{W})$: max $\int \rho(\hat{W}) \ln(\rho(\hat{W})/\rho_i(\hat{W})) dv$ proposed by Park and Band (1977). The first one has been inspected in § 3 while the second one, with an appropriately normalised density $\rho_i(\hat{W})$ (cf equation (5)) will result in $\rho_i(\hat{W})$. In this approach only one property of an initial $\rho(\hat{W})$ is unavoidable, namely any sensible

 $\rho(\hat{W})$ must satisfy that all $\mu(\alpha)$ are equal and this will be the case if and only if $\rho(\hat{W}) = \rho(\hat{U}\hat{W}\hat{U}^{+})$ for every \hat{U} and every \hat{W} i.e. when $\rho(\hat{W})$ is unitarily invariant.

Further specification of an initial 'complete ignorance' density should follow from possible information concerning the origin of the inspected ensemble. If for example an ensemble is the result of a preparation $\rho(\hat{W}) \sim S(\hat{W})$ is an extremely well founded choice; if on the other hand the inspected ensemble is a subensemble of decay products (an improper mixture, cf d'Espagnat, 1976) an initial density $\rho(\hat{W}) \sim (\det(\hat{W}))^k$ will be, perhaps, more appropriate.

5. Four examples

In this section we will examine four examples of some simple and 'natural' densities and their consequences.

(1) $\rho(\hat{W}) = \delta(\hat{W} - \hat{W}_0)$. In this case $\hat{W}_{RS}^E = \hat{W}_0$ and this density in fact corresponds to the preparation of \hat{W}_0 i.e. to the complete information concerning the inspected ensemble. In some $V_W(\{\hat{P}_k\})$, $\delta(\hat{W} - \hat{W}_0)$ will induce $\mu(\hat{W}) = \delta(\hat{W} - \hat{W}_0)$ where $\hat{W}_0' = \sum_k \hat{P}_k \hat{W}_0 \hat{P}_k$.

(2) $\rho(\hat{W}) = \rho(\hat{U}\hat{W}\hat{U}^+) \forall \hat{W} \in V_W, \forall \hat{U}, \hat{U}\hat{U}^+ = \hat{I}$. As already stated, this property is a necessary part of any initial 'complete ignorance' density. In this case marginal densities in two different subspaces $V_h(\{\hat{P}_k\})$ and $V_h(\{\hat{P}_k\})$ will be

$$\mu(\alpha_1,\ldots,\alpha_n) = \int \rho(\boldsymbol{\alpha}) \, \mathrm{d}\boldsymbol{\alpha}_{k>n} \text{ and } \mu(\boldsymbol{\beta}) = \int \rho(\boldsymbol{\beta}) \, \mathrm{d}\boldsymbol{\beta}_{k>n}$$

where $\boldsymbol{\alpha} = \{\alpha_1, \ldots, \alpha_n^2\}$ are coordinates in the basis in V_h induced by $\{\hat{P}_k\}$ while $\boldsymbol{\beta} = \{\beta_1, \ldots, \beta_n^2\}$ are coordinates in the basis induced by $\{\hat{P}_k\}$ (cf equation (1)). Due to the fact that $\rho(\hat{W}) = \rho(\hat{U}\hat{W}\hat{U}^+), \mu(\alpha) = \mu(\beta)$ whenever $\alpha = \beta$. Also if $\hat{U}\hat{P}_k\hat{U}^+ = \hat{P}'_k$ then $\hat{U}\hat{W}_M^E\hat{U}^+ = \hat{W}_M^E$, where \hat{W}_M^E is the expected state in $V_W(\{\hat{P}_k\})$ and \hat{W}_M^E , in $V_W(\{\hat{P}_k\})$. On the other hand all expected states \hat{W}_M^E are projections of a single \hat{W}_{RS}^E . The only state satisfying this condition i.e. that all its projections are unitarily equivalent is $\hat{W} = (1/n)\hat{I}$, hence for any unitarily invariant density $\rho(\hat{W})\hat{W}_{RS}^E = \hat{W}_M^E = (1/n)\hat{I}$.

An initial 'complete ignorance' density may be e.g. $\rho(\hat{W}) = (v(V_W))^{-1} \forall \hat{W} \in V_W$ where $v(V_W)$ is the volume of V_W (calculated of course in the hyperplane $h(\hat{A}|\text{Tr}(\hat{A}) = 1)$.

There is an interesting property of the unitarily equivalent densities when V_W^{ad} is the result of measurements and when V_W^{ad} is also unitary invariant i.e. $\hat{U}V_W^{ad}\hat{U}^+ = V_W^{ad}$, for some non-trivial \hat{U} . In such case the most probable state and the expected state will coincide.

(3) In this example we will reconsider a composite system ensemble. Every system is composed out of two subsystems, each one described in a three-dimensional vector space, e.g. H_1 and H_2 . The system is then described in $H_1 \otimes H_2$. For simplicity, we will assume that

(a) the unknown state is a pure one,

(b) that $[\mathrm{Tr}_1(\hat{P}^{(12)}), \hat{A}_0^{(2)}] = 0.$

(the set of states defined by (a) and (b) will be denoted V_0), and

(c) all states from V_0 are equally probable.

The measurements will be performed on the ensemble of first ('1') subsystems and the task will be to find a RS in $V_w^{(1)}$.

Now, let the measurements obtained in $V_W^{(1)ad}$ defined by

$$\hat{W}(\alpha) = \frac{1}{3}(\hat{P}_{1}^{(1)} + \hat{P}_{2}^{(1)} + \tilde{P}_{3}^{(1)}) + \frac{1}{3}(\hat{\sigma}_{12}^{(1)r} + \hat{\sigma}_{23}^{(1)r}) + \alpha\hat{\sigma}_{13}^{(1)r}.$$
(8)

The set $V_W^{(1)ad}$ defined by (8) is the segment of which the extremal points are $\hat{W}(0)$ and $\hat{W}((\frac{2}{9})^{-1/2})$. By $|w_k(\alpha)\rangle$ and $w_k(\alpha)$ we will denote eigenvectors and eigenvalues of $\hat{W}(\alpha)$. Then $\hat{W}(\alpha) = \text{Tr}_2(P_{(\alpha)}^{(12)})$ where $\hat{P}_{(\alpha)}^{(12)}$ is the projector on the vector

$$|\psi_{(\alpha)}^{(12)}\rangle = \sum_{k} \left(w(\alpha)_{k}\right)^{1/2} \exp(\mathrm{i}\phi_{k}) |w_{k}(\alpha)\rangle \otimes |a_{0k}\rangle$$

where $|a_{0k}\rangle$ are eigenvectors of the observable $\hat{A}_{0}^{(2)}$ from (b) while ϕ_{k} are variables. Condition (c) will give that $\rho(\hat{W}(\alpha)) = \rho(\alpha)$ is proportional to the volume of states in $V_{W}^{(12)}$ which will reduce into $\hat{W}(\alpha)$. In this case the volume is in fact a surface similar to a torus. After simple calculation one obtains

$$\rho(\alpha) = \text{constant} \times (\Sigma_k w_k(\alpha)) \left(\prod_k w_k(\alpha)\right)^{1/2}$$
$$\sim (\alpha ((2/9)^{1/2} - \alpha))^{1/2},$$

so that $\hat{W}_{RS}^E = \int W(\alpha)\rho(\alpha) \, d\alpha = \hat{W}(\alpha = (18)^{-1/2})$. On the other hand the maximum entropy state is $\hat{W}(\alpha \approx 0, 147)$.

(4) In the last example we will assume that V_W^{ad} is given through an inequality e.g. $\langle \hat{s}_z \rangle \ge 0$ for a spin $\frac{1}{2}$ particle. The maximum entropy RS will be $\hat{W} = \frac{1}{2}\hat{I}$ while the expected state $\hat{W}_{RS}^E = \frac{11}{16}\hat{P}(z, +) + \frac{5}{16}\hat{P}(z, -)$ assuming that all states \hat{W} satisfying $Tr(\hat{W}\hat{s}_z) \ge 0$ are equally probable.

These examples should show that the difference between the most probable state and an expected state may occur in some simple examples. Example (3) shows that a density different from $\rho(\hat{W}) \sim S(\hat{W})$ will occur when an ensemble of the correlated subsystems is inspected. In (4) the most probable state lies on the boundary of V_{W}^{ad} , which will never occur with an expected state, still a decisive, general answer on the question 'When to use the most probable state and when to use an expected state?' is not given in this note. Namely, such an answer will be possible only if a better knowledge of a stochasticity in the inspected ensemble can be obtained. However, it is possible to identify two extremal cases: if the results obtained from the measurements are assumed to be the result of a single trial the most probable state will be the more appropriate choice; if, on the other hand the same set of procedures is assumed to be a set of repeated trials, an expected state will be more appropriate.

6. Summary

The inspected, expected Rs, may be useful as an alternative to the most probable Rs of which equation (3) is the most frequent case. As already stated the choice between these Rss will be much easier if a better understanding of an inspected ensemble is possible.

A serious obstacle concerning an expected Rs is the fact that it is much easier to obtain the most probable Rs than an expected state. Nevertheless a proper quantal approach to this problem can hardly avoid such difficulties.

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