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Perturbations and Non-Normalizable Eigenvectors

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Abstract. A spectral representation of a self-adjoint operator acting in a Hilbert space is given by eigenvectors of an extension of the operator to a suitable space containing the original Hilbert space. A perturbation argument shows the extended operator has no eigenvalues that do not belong to the spectrum of the original operator. The abstract result is applied to Schrödinger operators $-\Delta + V$.

1. Introduction

The spectral theory of self-adjoint operators may be treated without ever mentioning non-normalizable eigenvectors. In fact, the spectral theorem may be stated as follows [1].

Theorem. Let A be a self-adjoint operator acting in the Hilbert space H. Then A is unitarily equivalent to a multiplication operator. That is, there is a Hilbert space $L^2(M, \mu)$, a real measurable function α on M, and a unitary operator $U : H \to L^2(M, \mu)$ such that f is in the domain of A if and only if $\alpha\, U f$ is in $L^2(M, \mu)$, and such that $U A f = \alpha\, U f$.

Here μ is a positive measure and $L^2(M, \mu)$ is the Hilbert space of all measurable complex functions h on M such that $\int | h(p) |^2 \, d\mu(p) < \infty$. (Functions which are equal almost everywhere are identified.) Such a unitary equivalence of A with a multiplication operator is called a spectral representation of A. The spectral theorem asserts the existence but not the uniqueness of spectral representations.

Let ϕ be a Borel measurable function defined on the real numbers. Then $\phi(A)$ may be defined by the spectral theorem as the operator acting in H which is unitarily equivalent to multiplication by $\phi(\alpha)$ [1]. This definition is independent of the spectral representation.

Non-normalizable eigenvectors enter the picture only when one attempts to describe the form of the unitary operator U. A suitable space K^* containing H is chosen. Vectors in K^* which are not in H are called non-normalizable vectors. (The norm under consideration is that of H, of course.) The self-adjoint operator A acting in H has an extension to an operator $\tilde{A}$ acting in K^*. When A has continuous spectrum U is given in terms of non-normalizable eigenvectors of $\tilde{A}$.

G. I. Kac has given an elegant criterion for showing that K^* is large enough to contain all the non-normalizable eigenvectors necessary for any spectral representation [2]. It is desirable to choose K^* as small as possible consistent with this requirement, since this allows the widest class of perturbations and gives the sharpest estimates on non-normalizable eigenvectors. Also, if K^* is reasonably small, the eigenvalues of $\tilde{A}$ may give a good idea of the spectrum of A. (In general, since $\tilde{A}$ acting in K^* is not self-adjoint, it may even have non-real eigenvalues.) Here an abstract perturbation theory is developed to show that K^* does not contain unwanted non-normalizable eigenvectors of $\tilde{A}$. This is applied to Schrödinger operators $-\Delta + V$. In this case the results may be interpreted as estimates on growth at infinity of eigenfunctions of the Schrödinger operator. (Such results have also been obtained by partial differential equations methods [3].) Much stronger assumptions on the interaction would be needed in order to apply the theory of wave operators and scattering.

2. Non-Normalizable Eigenvectors

Let H be a Hilbert space. The inner product of g and f in H will be denoted $\langle g, f\rangle$. The convention adopted here is that the inner product is conjugate linear in the first variable and linear in the second variable. The norm of f in H is $\|f\| = \langle f, f\rangle^{1/2}$.

We wish to consider a situation where there is given another Hilbert space K which is a dense linear subspace of H. If f is an element of K, the norm of f as an element of K is written $\|f\|_K$. We shall assume that the injection of K into H is continuous. Thus there is a constant $c > 0$ such that $\|f\| \leqslant c\|f\|_K$.

Let K^* be the set of all bounded linear functions from K to the complex numbers.

Proposition 1. Let H be a Hilbert space. Let $K \subset H$ be another Hilbert space. Assume that K is dense in H and that the injection is continuous. To each g in H associate the linear function $f \to \langle g, f\rangle$ in K^*. Then this correspondence is injective, and H may be identified with a dense subspace of K^*, so that we have continuous inclusions of Hilbert spaces $K \subset H \subset K^*$.

Proof: If g is an element of H, then $|\langle g, f\rangle| \leqslant \|g\| \, \|f\| \leqslant c\|g\| \, \|f\|_K$, so the function which assigns to f in K the inner product $\langle g, f\rangle$ is in K^*. If the inner product $\langle g, f\rangle = 0$ for all f in K, then $g = 0$, since K is dense in H. Thus each element g in H determines a unique element of K^*. We identify each g in H with the corresponding element of K^*.

We wish to give K^* the structure of a Hilbert space in such a way that the injection of H into K^* is linear. If ψ is in K^* and f is in K, we write $\langle \psi, f\rangle$ for the value of ψ on f. If ψ_1 and ψ_2 are in K^*, we define $\psi_1 + \psi_2$ by $\langle \psi_1 + \psi_2, f\rangle = \langle \psi_1, f\rangle + \langle \psi_2, f\rangle$. If ψ is in K^* and a is a complex number, it is convenient to define the product of a with ψ to be given by $\langle a\,\psi, f\rangle = a^* \langle \psi, f\rangle$. With this convention, if ψ happens to be in H this coincides with scalar multiplication in H. With the definition $\|\psi\|_{K^*} = \sup\{|\langle \psi, f\rangle| : \|f\|_K \leqslant 1\}$, K^* becomes a Hilbert space.

Note that we have $\|g\|_{K^*} = \sup\{|\langle g, f\rangle| : \|f\|_K \leqslant 1\} \leqslant c \sup\{|\langle g, f\rangle| : \|f\| \leqslant 1\} = c\|g\|$. Hence the inclusion of H into K^* is continuous. It is also not hard to see that H is dense in K^*. This completes the proof.

Warning: Having identified $H \subset K^*$, it is no longer permissible to identify K^* with K.

Definition. Let H be a Hilbert space and let $K \subset H$ be another Hilbert space. Assume that K is dense in H and that the inclusion is continuous. Then the triple $K \subset H \subset K^*$ will be called a scale of Hilbert spaces.

From now on we shall assume that all Hilbert spaces under consideration have a countable orthonormal basis. (This is equivalent to their being separable metric spaces.) This allows us to consider only measure spaces which are σ-finite.

We now recall the theorem of Kac [2].

Theorem 1. Let A be a self-adjoint operator acting in H. Assume that $U: H \to L^2(M, \mu)$ is a unitary operator which gives a spectral representation of A. Let $K \subset H \subset K^*$ be a scale of Hilbert spaces. Assume that there is a Borel measurable function β which is bounded on the spectrum of A and which does not vanish on the spectrum of A such that $\beta(A)$ is a Hilbert-Schmidt operator from K to H. Then there is a function ψ from M to K^* such that for every f in K, $Uf\,(p) = \langle \psi(p), f\rangle$ for almost every p in M.

For the convenience of the reader we sketch a proof.

Proof: $U\,\beta(A) = \beta(\alpha)\;U: K \to L^2(M, \mu)$ is a Hilbert-Schmidt operator. Represent K as a space $L^2(N, \nu)$. Then there is an s in $L^2(M \times N, \mu \times \nu)$ such that for f in K, $\beta(\alpha(p))\;Uf\,(p) = \int s(p, q)\,f(q)\,d\nu(q)$ for almost every p [4]. By Fubini's theorem, $s(p, q)$ is in $L^2(N, \nu)$ as a function of q for almost every p. Thus for these p we may define $\langle \psi(p), f\rangle = \big(1/\beta(\alpha(p))\big) \int s(p, q)\,f(q)\,d\nu(q)$. $\psi(p)$ is in K^* by the Schwarz inequality.

Remark. In practice the most useful choices of β are $\beta(a) = (a - z)^{-k}$ for some integer $k = 1, 2, 3, \ldots$ and z not in the spectrum of A. Another possibility is $\beta(a) = 1$. In this case the condition is simply that the injection of K into H is Hilbert-Schmidt.

Note. If f and g are in H, and f is in the domain of A, we have

$$\langle g, A f\rangle = \int Ug\,(p)^*\,\alpha(p)\;Uf\,(p)\;d\mu(p)\,.$$

In particular, under the conditions of Theorem 1, if f and g are in K, $\langle g, A f\rangle = \int \langle g, \psi(p)\rangle\,\alpha(p)\,\langle \psi(p), f\rangle\,d\mu(p)$. (In keeping with the usage in physics, we have written $\langle g, \psi(p)\rangle$ for $\langle \psi(p), g\rangle^*$.)

Definition. Let $K \subset H \subset K^*$ be a scale. Let A be a self-adjoint operator acting in H with domain D. Let $D_0 = \{f \text{ in } K \cap D : A f \text{ is in } K\}$. Assume D_0 is dense in K. Then the scale extension $\tilde{A}$ of A is defined as the operator acting in K^* which is the adjoint of A restricted to D_0.

Explicitly, if g is in K^*, g is in the domain of $\tilde{A}$ if there is an h in K^* with $\langle h, f\rangle = \langle g, A f\rangle$ for all f in D_0. Since D_0 is dense in K, h is uniquely determined and we set $\tilde{A}\,g = h$. $\tilde{A}$ is clearly an extension of the original self-adjoint operator A.

Theorem 2 [2]. Let A be a self-adjoint operator acting in H. Let $K \subset H \subset K^*$. Let U be a spectral representation of A and assume that there is a function ψ from M to K^* such that $(U f)\,(p) = \langle \psi(p), f\rangle$ for almost every p in M. Assume that the scale extension $\tilde{A}$ of A is defined. Then $\psi(p)$ is in the domain of definition of $\tilde{A}$ and $\tilde{A}\psi(p) = \alpha(p)\psi(p)$ for almost every p.

Proof: Let f be in D_0. Then $\langle\psi(p), Af\rangle = UAf(p) = \alpha(p)\,Uf(p) = \langle\alpha(p)\psi(p), f\rangle$ for almost every p. Thus for any countable subset of D_0, $\langle\psi(p), Af\rangle = \langle\alpha(p)\psi(p), f\rangle$ for f in the subset for almost every p. Now the graph of the operator A restricted to D_0 is a subspace of the direct sum of K with itself. Since a subspace of a separable metric space is separable, the graph is separable. Thus there is a countable subset of D_0 such that for each f in D_0, there is a subsequence f_n in the subset with $f_n \to f$ and $Af_n \to Af$, in the norm of K. We conclude that $\langle\psi(p), Af\rangle = \langle\alpha(p)\psi(p), f\rangle$ for all f in D_0 for almost every p. In other words, for these p, $\tilde{A}\psi(p) = \alpha(p)\psi(p)$.

3. Perturbation Theory

Theorem 3. Let $K \subset H \subset K^*$ be a scale of Hilbert spaces. Let A be a self-adjoint operator acting in H. Assume that $(A - z)^{-1}$ is a Hilbert-Schmidt operator from K to H for some z not in the spectrum of A. Assume that B is a self-adjoint operator whose domain contains the domain of A and such that $A + B$ is self-adjoint with the same domain as A. Then if z is also not in the spectrum of $A + B$, $(A + B - z)^{-1}$ is a Hilbert-Schmidt operator from K to H.

Proof: The two resolvents are related by
$(A + B - z)^{-1} = [1 - (A + B - z)^{-1}B]\,(A - z)^{-1}$. Let T be the closure of $1 - (A - B - z)^{-1}B$. Then its adjoint $T^* = 1 - B(A + B - z^*)^{-1}$. Since $A + B$ has the same domain as A, T^* is defined on all of H. But any adjoint has a closed graph. So T^* is a bounded operator from H to H, by the closed graph theorem. Hence T is also bounded from H to H. The identity $(A + B - z)^{-1} = T(A - z)^{-1}$ thus exhibits $(A + B - z)^{-1}$ as a Hilbert-Schmidt operator from K to H followed by a bounded operator from H to H.

Proposition 2. Let A be a self-adjoint operator acting in the Hilbert space H. Let $K \subset H \subset K^*$ be a scale of Hilbert spaces. Assume that the scale extension of A to an operator $\tilde{A}$ acting in K^* exists. Let λ be a complex number which is not in the spectrum of A. Then if $(A - \lambda)^{-1}$ sends K into K, λ is not an eigenvalue of $\tilde{A}$.

Proof: Assume that $(\tilde{A} - \lambda)\,\psi = 0$ for some ψ in K^*. If $(A - \lambda)^{-1}$ sends K into K, then the range of $A - \lambda$ restricted to D_0 is K. Hence $\langle\psi, (A - \lambda)f\rangle = 0$ for f in D_0 implies $\psi = 0$.

Definition. Let T be a positive self-adjoint operator acting in H with bounded inverse $T^{-1}\colon H \to H$. For $0 \leqslant s < \infty$, let K_s be the domain of T^s with the norm $\|f\|_s = \|T^s f\|$. Then the family $K_s \subset H \subset K_s^*$, $0 \leqslant s < \infty$, of scales is called an analytic scale.

There are interpolation theorems which apply to analytic scales. We shall need only the following special case [5].

Proposition 3. Let the spaces $K_s \subset H$, $0 \leqslant s < \infty$, define an analytic scale. Let $R\colon H \to H$ be a bounded operator and assume that it has a bounded restriction $R\colon K_a \to K_a$. Then $R\colon K_s \to K_s$ is bounded for $0 \leqslant s \leqslant a$.

Theorem 4. Let H be a Hilbert space. Let A be a self-adjoint operator acting in H with domain D. Let B be a self-adjoint operator acting in H whose domain contains D. Assume that $A + B$ is self-adjoint on D. Let the spaces $K_s \subset H$, $0 \leqslant s < \infty$, determine an analytic scale and set $K_1 = K$. Assume that for some $\varepsilon > 0$ and all s, $0 \leqslant s \leqslant 1$, $B: D \cap K_s \to K_{s+\varepsilon}$ is bounded. Then if λ is not in the spectrum of A or of $A + B$, and if the restriction $(A - \lambda)^{-1}: K \to K$ is bounded, then the restriction $(A + B - \lambda)^{-1}: K \to K$ is bounded.

Proof: We have $K = K_1 \subset K_s \subset K_0 = H$ for $0 \leqslant s \leqslant 1$. The space $D \cap K_s$ may be given the norm $(\| A f \|^2 + \| f \|_s^2)^{1/2}$, where $\| f \|_s$ is the norm on K_s.

Write
$$(A + B - \lambda)^{-1} = \sum_{n=0}^{r-1} (-1)^n \left((A - \lambda)^{-1} B\right)^n (A - \lambda)^{-1} + (-1)^r \left((A - \lambda)^{-1} B\right)^r (A + B - \lambda)^{-1}.$$
Consider the first r terms in the sum. Since $(A - \lambda)^{-1}: K \to D \cap K$ and $B: K \cap D \to K$ are bounded, each term is bounded from K to $D \cap K \subset K$.

To treat the final term in the sum, we use interpolation. Since $(A - \lambda)^{-1}: H \to H$ and $(A - \lambda)^{-1}: K \to K$ are bounded, it follows from Proposition 3 that $(A - \lambda)^{-1}: K_s \to K_s$ is bounded for $0 \leqslant s \leqslant 1$. Take r so large that $1/r < \varepsilon$. Then $B: D \cap K_{(n-1)/r} \to K_{n/r}$ is bounded, $n = 1, 2, 3, \ldots, r$. Since $(A - \lambda)^{-1}: K_{n/r} \to D \cap K_{n/r}$ and $(A + B - \lambda)^{-1}: H \to D$ are bounded, the final term is bounded from $H \supset K$ to $D \cap K \subset K$.

4. Schrödinger Operators

Let $H = L^2(\boldsymbol{R}^3, dx)$. Let $\varrho \geqslant 0$ be a real function on $\boldsymbol{R}^3$ which is bounded and never zero. Let $K = L^2(\boldsymbol{R}^3, \varrho(x)^{-1}\, dx)$. Then $K \subset H$, the injection is continuous, and K is dense in H. So $K \subset H \subset K^*$ is a scale of Hilbert spaces. The nice feature of this case is that K^* has a natural realization as a space of functions. It should be considered as $K^* = L^2(\boldsymbol{R}^3, \varrho(x)\, dx)$. Then if g is in K^* and f is in K, $\langle g, f\rangle = \int g(x)^* f(x)\, dx$ and $|\langle g, f\rangle| \leqslant \| g \|_{K^*} \| f \|_K$.

In the following we shall require that ϱ be bounded away from zero on compact sets. This ensures that the K, H, and K^* norms are equivalent on any set of f with fixed compact support.

Example. Consider the Laplace operator Δ. Δ is a self-adjoint operator acting in H and one spectral representation is given by the Fourier transform $F: H \to L^2(\boldsymbol{R}^3, (2\pi)^{-3}\, dk)$. $(F \Delta f)(k) = -k^2 F f(k)$, so Δ is isomorphic to multiplication by $\alpha(k) = -k^2$. Assume now that ϱ is in $L^1(\boldsymbol{R}^3, dx)$. Notice that for f in K, $(F f)(k) = \int \exp(-i\,k\,x) f(x)\, dx = \langle \psi(k), f\rangle$, where $\psi(k)$ is the function $\exp(i\,k\,x)$ in K^*. The $\psi(k)$ are non-normalizable eigenvectors: $\Delta \exp(i\,k\,x) = -k^2 \exp(i\,k\,x)$.

Definition. Let V be a real function on $\boldsymbol{R}^3$ such that $V = V_1 + V_2$, where V_1 is in $L^\infty(\boldsymbol{R}^3, dx)$ and V_2 is in $L^2(\boldsymbol{R}^3, dx)$. Then V will be said to satisfy the Kato condition.

Proposition 4 [6]. Let $H = L^2(\boldsymbol{R}^3, dx)$. Assume that V is a real function on $\boldsymbol{R}^3$ which satisfies the Kato condition. Then $-\Delta + V$ is a self-adjoint operator acting in H with the same domain as that of $-\Delta$.

Theorem 5. Let $\varrho \geqslant 0$ be a function on $\boldsymbol{R}^3$ which is bounded on $\boldsymbol{R}^3$ and bounded away from zero on compact subsets of $\boldsymbol{R}^3$. Assume that ϱ is in $L^1(\boldsymbol{R}^3, dx)$. Let $K \subset H \subset K^*$ be the scale $L^2(\boldsymbol{R}^3, \varrho(x)^{-1}\, dx) \subset L^2(\boldsymbol{R}^3, dx) \subset L^2(\boldsymbol{R}^3, \varrho(x)\, dx)$. Let V be a real function on $\boldsymbol{R}^3$ which satisfies the Kato condition. Then for any spectral representation $U: H \to L^2(M, \mu)$ of $-\Delta + V$ there is a function ψ from M to K^* such that for each f in K, $(U f)(p) = \langle \psi(p), f \rangle$ for almost every p in M. The $\psi(p)$ are (possibly non-normalizable) eigenvectors of the scale extension of $-\Delta + V$ for almost every p in M.

Proof: If $z > 0$, $(z - \Delta)^{-1}$ is an integral operator acting in H with kernel $(4\pi\,|\,x - y\,|)^{-1} \exp(-z^{1/2}\,|\,x - y\,|)$. Now $(4\pi\,|\,x - y\,|)^{-1} \exp(-z^{1/2}\,|x - y|)\,\varrho(y)^{1/2}$ is in $L^2(\boldsymbol{R}^6, dx\, dy)$. Hence it is the kernel of a Hilbert-Schmidt operator from H to H. Next note that multiplication by $\varrho^{-1/2}$ is an isomorphism from K to H. It follows that $(z - \Delta)^{-1}$ is a Hilbert-Schmidt operator from K to H.

If $z > 0$ is sufficiently positive, then $-z$ will not be in the spectrum of $-\Delta + V$ [6]. Hence Theorem 3 implies that $(z - \Delta + V)^{-1}$ is Hilbert-Schmidt from K to H. Thus Theorem 1 applies to $-\Delta + V$.

We now show that $-\Delta + V$ has a scale extension. First note that the $L^2(\boldsymbol{R}^3, dy)$ norm of $(4\pi\,|\,x - y\,|)^{-1} \exp(-z^{1/2}\,|\,x - y\,|)$ is finite and independent of x. It follows that $(z - \Delta)^{-1} g$ is in $L^\infty(\boldsymbol{R}^3, dx)$ for g in H. Hence the domain of definition of Δ is contained in $L^\infty(\boldsymbol{R}^3, dx)$. Now consider the space D_1 of functions in the domain of Δ which have compact support. Clearly D_1 is dense in K. $-\Delta$ sends D_1 into K. Multiplication by V_1 leaves K invariant. On the other hand, since the domain of Δ is contained in $L^\infty(\boldsymbol{R}^3, dx)$, multiplication by V_2 sends D_1 into K. Thus $-\Delta + V$ sends the dense set D_1 into K. This implies that the scale extension of $-\Delta + V$ exists and hence that Theorem 2 applies.

Surprisingly, Theorem 5 does not imply that the non-normalizable eigenfunctions are bounded. The exceptional set of p in M for which the $\psi(p)$ are not eigenvectors in K^* will depend in general on the choice of the scale. Maslov [7] has given an example of a bounded continuous V for which the non-normalizable eigenfunctions for some interval of energy are unbounded at infinity. Berezanskii [8] has given estimates on their rate of increase.

In the following we write $r = |\,x\,|$.

Definition. Let V be a real measurable function on $\boldsymbol{R}^3$. Assume that $V = V_1 + V_2$, where $|\,V_1(x)\,| \leqslant c(1 + r^2)^{-\varepsilon/2}$ for some $\varepsilon > 0$ and some c, and V_2 is in $L^2(\boldsymbol{R}^3, dx)$ and has compact support. Then V will be said to satisfy the condition of slight decrease.

Note that a function V of slight decrease satisfies the Kato condition. In addition it is a relatively compact perturbation of $-\Delta$, so that the essential spectrum of $-\Delta + V$ is $[0, \infty)$ [9]. In particular, the spectrum of $-\Delta + V$ contains the spectrum of $-\Delta$.

A particularly convenient choice of the function ϱ defining the scale is $\varrho(x) = (1 + r^2)^{-s/2}$, $s \geqslant 0$. The condition that ϱ is in $L^1(\boldsymbol{R}^3, dx)$ is satisfied provided $s > 3$.

Theorem 6. Fix s, $0 \leqslant s < \infty$. Let $K_s \subset H \subset K_s^*$ be the scale $L^2(\boldsymbol{R}^3, (1 + r^2)^{s/2}\, dx) \subset L^2(\boldsymbol{R}^3, dx) \subset L^2(\boldsymbol{R}^3, (1 + r^2)^{-s/2}\, dx)$. Let V be a real function on $\boldsymbol{R}^3$ which satisfies the condition of slight decrease. Then the scale extension of $-\Delta + V$ to an operator in K_s^* has the complex number λ as an eigenvalue only if λ is real and in the spectrum of the self-adjoint operator $-\Delta + V$ acting in H.

Proof: Let T be the operator given by multiplication by $(1 + r^2)^{1/4}$. Then the scale in the theorem is the analytic scale associated with T; K_s is the domain of T^s, $s \geqslant 0$.

In order to apply Theorem 4 we first show that for $z > 0$ or z not real, $(z + \Delta)^{-1}$: $K_s \to K_s$ is continuous, $s \geqslant 0$. Start with the case when s is an integer multiple of 4, $s = 4k$. By taking Fourier transforms we see that this is equivalent to showing that $(z - k^2)^{-1}$ is a continuous multiplication operator from $D(\Delta^k)$ to $D(\Delta^k)$. For f in $D(\Delta^k)$, expand $\Delta^k\big((z - k^2)^{-1} f\big)$ as a sum of products of partial derivatives of $(z - k^2)^{-1}$ and of f. The partial derivatives of f can be estimated in L^2 norm in terms of $\| \Delta^k f \|_2$ and $\| f \|_2$. On the other hand, the partial derivatives of $(z - k^2)^{-1}$ are all bounded functions (since they are Fourier transforms of integrable functions). Thus we have an estimate on $\| \Delta^k\big((z - k^2)^{-1} f\big) \|_2$, which disposes of the case when k is an integer. The general case now follows from Proposition 3.

The other hypothesis of Theorem 4 follows from the assumption of slight decrease. Multiplication by V_1 is bounded from K_s to $K_{s+\varepsilon}$ for some $\varepsilon > 0$. On the other hand, V_2 is bounded from D to K_s for all $s \geqslant 0$, since $D \subset L^\infty(\mathbf{R}^3, dx)$ and V_2 has compact support. Thus $V: K_s \cap D \to K_{s+\varepsilon}$ is bounded.

So if λ is not in the spectrum of $-\Delta + V$, $(-\Delta + V - \lambda)^{-1}: K_s \to K_s$ is bounded. The theorem then follows from Proposition 2.

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