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On the Derivation of the Schroedinger Equation in a Riemannian Manifold

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Abstract. Under certain conditions it is shown that the kinetic part of the dynamical operator of a quantum mechanical system with a Riemannian manifold as configuration space is the Laplace-Beltrami operator.

§ 1. Introduction

In his book on the "Mathematical foundations of quantum mechanics" [2]. MACKEY raises the problem of characterising the kinetic part of the Schroedinger equation in a Riemannian manifold. The main aim of this paper is to show that under certain conditions the dynamical operator of a quantum mechanical system with a Riemannian manifold as its configuration space has its kinetic part locally unitarily equivalent to the Laplace-Beltrami operator. Since in a Riemannian manifold there need not exist one parameter groups of isometries it seems necessary to characterise the Schroedinger operator without using the notion of momentum. In the case of Euclidean configuration space MACKEY obtains the kinetic part of the Schroedinger operator by equating the velocity operator to a constant multiple of the momentum operator. Instead we start from the assumption that the acceleration operator is equal to a constant times the force operator.

In general notations and terminology we follow [2]. Regarding the basic properties of Riemannian manifolds and notations of tensor calculus we refer to [1].

§ 2. Quantum Mechanical Systems with one Degree of Freedom

Let R denote the real line and $L_2(R)$ the space of all complex valued functions on R square integrable with respect to the Lebesgue measure. For any complex valued function g on R we shall denote by $g^{(r)}$ the r-th. derivative of g. We shall adopt the notation g for both the function g as well as multiplication by g. For any two operators A and B of $L_2(R)$ into itself we shall denote by $[A, B]$ the operator $AB - BA$.

Let H be the dynamical operator of a quantum mechanical system whose state vectors are unit vectors in $L_2(R)$. If x denotes the position operator, then $i[H, x]$ is the velocity operator and $-[H, [H, x]]$ is the acceleration operator.

We shall now derive the form of H under the assumption that the acceleration operator is a multiplication operator and an energy equation is satisfied.

Theorem 2.1. *Let H be a symmetric differential operator with twice differentiable coefficients and*

a) $$m[H, [H, x]] = - v^{(1)}$$

b) $$m[H, [H, x]^2] = c[H, v],$$

where m and c are non zero constants and v is an infinitely differentiable function. Suppose $v^{(3)}$ does not vanish on a set of positive Lebesgue measure. Then $c = -2$ and H is a second order differential operator which is unitarily equivalent to an operator of the form $h\frac{d^2}{dx^2} + \frac{v}{2hm} + \alpha$ where h and α are constants. The unitary equivalence can be effected through a multiplication operator.

Proof. Condition b) implies that

$$m[H, x][H, [H, x]] + m[H, [H, x]][H, x] = c[H, v].$$

By condition a) we have

$$[H, x]v^{(1)} + v^{(1)}[H, x] = -c[H, v]. \tag{2.1}$$

Suppose

$$H = a_n \frac{d^n}{dx^n} + a_{n-1}\frac{d^{n-1}}{dx^{n-1}} + \cdots + a_0$$

where $a_n \neq 0$. By applying the operators on either side of (2.1) to C^∞ functions with compact supports and equating the coefficients of $\frac{d^k}{dx^k}$, $0 \leqq k \leqq n-1$, we have

$$(k+1)a_{k+1}v^{(1)} + \sum_{r=k+1}^{n} r a_r \binom{r-1}{k} v^{(r-k)} = -c \sum_{r=k+1}^{n} a_r \binom{r}{k} v^{(r-k)}.$$

Putting $k = n-1$, we get

$$2na_n v^{(1)} = -cna_n v^{(1)}.$$

Since $v^{(1)} \neq 0$, $c = -2$. Putting $k = n-3$, we have

$$\binom{n}{3} a_n v^{(3)} = 0.$$

Since $v^{(3)} \neq 0$ and $a_n \neq 0$, we have $\binom{n}{3} = 0$. I.e., $n \leqq 2$. In other words H is a second order differential operator.
Suppose

$$H = a\frac{d^2}{dx^2} + b\frac{d}{dx} + d.$$

Substituting this operator in condition (a), we obtain

$$m\left\{2aa^{(1)}\frac{d^2}{dx^2} + (2aa^{(2)} + 2ba^{(1)})\frac{d}{dx} + ab^{(2)} + bb^{(1)} - 2ad^{(1)}\right\} = -v^{(1)}.$$

Thus $aa^{(1)} = 0$. In other words $a = h$ where h is a constant.

Further

$$m(hb^{(2)} + bb^{(1)} - 2hd^{(1)}) = - v^{(1)} .$$

Hence

$$d = \frac{1}{2h}(hb^{(1)} + b^2/_2 + v/m) + \alpha$$

where α is a constant. Thus

$$H = h\frac{d^2}{dx^2} + v/2hm + b\frac{d}{dx} + \frac{1}{2h}(hb^{(1)} + b^2/_2) + \alpha .$$

The symmetry of H implies that b is purely imaginary. Consider the unitary operator U defined by

$$Uf = f \exp\left[-\frac{1}{2h}\int_0^x b(t)\,dt\right] .$$

A simple calculation shows that

$$U^{-1}HU = h\frac{d^2}{dx^2} + \frac{v}{2hm} + \alpha .$$

This completes the proof.

Remark. Theorem 2.1 shows that one may take $\frac{h}{2m}\frac{d^2}{dx^2} + \frac{v}{h}$ as the most general dynamical operator of a quantum mechanical system with one degree of freedom. Condition (*b*) of the theorem can be written as

$$\left[H, -\frac{m}{2}[H,x]^2 - v\right] = 0$$

$-[H, x]^2$ is the square of the velocity operator and $-v$ is the potential energy operator.

§ 3. Systems with n Degrees of Freedom

We shall now consider a quantum mechanical system whose configuration space is the n-dimensional real Euclidean space R^n. Let H be the dynamical operator of the system acting in the Hilbert space $L_2(R^n)$ of complex valued functions square integrable with respect to the Lebesgue measure. In the preceding section we derived the form of H under the assumption that an energy equation is satisfied and the acceleration operator is a multiplication operator. We shall now replace the energy equation by the assumption that H is a second order differential operator. For any twice differentiable function φ we assume that $[[H, \varphi], \varphi] = 0$ if and only if φ is a constant. This assumption simply means that if a function of the position coordinates can be observed simultaneously with its rate of change, then it is a constant. We now have the following theorem.

Theorem 3.1. *Let H be a symmetric second order differential operator of the form*

$$H = \sum_{i,j} a_{ij} \frac{\partial^2}{\partial x_i \partial x_j} + \sum_i b_i \frac{\partial}{\partial x_i} + c$$

where a_{ij}, b_i and c are twice differentiable. Suppose for any twice differentiable function φ, the equation $[[H, \varphi], \varphi] = 0$ holds if and only if φ is a constant.

Let

$$m_i[H, [H, x_i]] = - V_i , \quad i = 1, 2 \ldots n \tag{3.1}$$

where V_i are once differentiable functions and m_i are constants. Then H is unitarily equivalent to an operator of the form

$$\sum_{i,j} a_{ij} \frac{\partial^2}{\partial x_i \partial x_j} + v$$

where $((a_{ij}))$ is a constant non singular positive or negative definite matrix such that

$$A^{-1} M^{-1} J = J' M^{-1} A^{-1} . \tag{3.2}$$

Here

$$A = ((a_{ij})) , M = ((m_i \delta_{ij})) , J = \left(\left(\frac{\partial V_i}{\partial x_j}\right)\right) ,$$

J' is the transpose of J and v is a function satisfying the equations

$$\sum_j a_{ij} \frac{\partial v}{\partial x_j} = \frac{V_i}{2m_i} . \tag{3.3}$$

The unitary equivalence here can be effected by a multiplication operator.

Conversely any operator of the form described above satisfies Eq. (3.1).

Remark 1. If there exists a function V such that $V_i = \frac{\partial V}{\partial x_i}$ for all i, then (3.2) and (3.3) are automatically satisfied if $A = \left(\left(- \frac{h}{2m_i} \delta_{ij}\right)\right)$ and $v = V$ where h is a constant. H then assumes the standard form

$$- \sum_i \frac{h}{2m_i} \frac{\partial^2}{\partial x_i^2} + \frac{V}{h} .$$

Proof of Theorem 3.1. First of all we observe that without loss of generality we may assume that $a_{ij} = a_{ji}$ for all i and j. The symmetry of H implies that the a_{ij} are all real. Since under coordinate transformations the a_{ij} behave like the coefficients of a second order symmetric contravariant tensor we may and do employ the standard notations of tensor calculus. In particular repeated index in a product implies that summation has been carried out. We shall denote $\frac{\partial a_{ij}}{\partial x_k}$ $\frac{\partial^2 a_{ij}}{\partial x_k \partial x_l}$ . . . by

$a_{ij,k}\, a_{ij,kl} \ldots$ respectively. Simple calculations show that

$$[H, x_i] = 2a_{ij}\frac{\partial}{\partial x_j} + b_i$$

$$\begin{aligned}[H, [H, x_i]] = {} & 2a_{kl}\left(a_{ir,k}\frac{\partial^2}{\partial x_l \partial x_r} + a_{ir,l}\frac{\partial^2}{\partial x_k \partial x_r}\right) - 2a_{ir}a_{kl,r}\frac{\partial^2}{\partial x_k \partial x_l} \\ & + 2a_{kl}a_{ir,kl}\frac{\partial}{\partial x_r} + a_{kl}\left(\frac{\partial b_i}{\partial x_l}\frac{\partial}{\partial x_k} + \frac{\partial b_i}{\partial x_k}\frac{\partial}{\partial x_l}\right) \\ & + 2\left(b_l a_{ir,l}\frac{\partial}{\partial x_r} - a_{ir}\frac{\partial b_l}{\partial x_r}\frac{\partial}{\partial x_l}\right) + a_{kl}\frac{\partial^2 b_i}{\partial x_k \partial x_l} \\ & + b_l\frac{\partial b_i}{\partial x_l} - 2a_{ir}\frac{\partial c}{\partial x_r}\end{aligned} \tag{3.4}$$

By (3.1), the coefficients of $\frac{\partial^2}{\partial x_k \partial x_l}$ and $\frac{\partial}{\partial x_k}$ in (3.4) must vanish. Hence

$$a_{rl}a_{ik,r} + a_{kr}a_{il,r} - a_{ir}a_{kl,r} = 0 \qquad \text{for every } i, k, l\,. \tag{3.5}$$

Interchanging i and k in (3.5) and adding to (3.5) we obtain

$$a_{rl}a_{ik,r} = 0 \qquad \text{for every } i, k, l\,. \tag{3.6}$$

If we put $\varphi = a_{ik}$ it follows from (3.6) that

$$[[H, \varphi], \varphi] = 2a_{rl}\frac{\partial\varphi}{\partial x_r}\frac{\partial\varphi}{\partial x_l} = 0\,.$$

Thus by hypothesis φ is a constant. In other words all the a_{ij} are constant. Let ψ by the linear function $c_i x_i$ where $c_1, c_2, \ldots, c_n$ are real constants. Then

$$[[H, \psi], \psi] = 2a_{ij}c_i c_j\,.$$

Hence the quadratic form $a_{ij}c_i c_j = 0$ if and only if all the c_i's are zero. Thus the constant matrix $((a_{ij}))$ is non singular and positive or negative definite. Hence its inverse exists and we shall denote it by $((a^{ij}))$.

Equating the coefficient of $\frac{\partial}{\partial x_k}$ in (3.4) to zero we have

$$a_{kl}\frac{\partial b_i}{\partial x_l} - a_{il}\frac{\partial b_k}{\partial x_l} = 0 \qquad \text{for every } i, k\,. \tag{3.7}$$

Putting $b^i = a^{ij}b_j$, we can rewrite (3.7) as

$$\frac{\partial b^i}{\partial x_j} = \frac{\partial b^j}{\partial x_i} \qquad \text{for every } i, j\,. \tag{3.8}$$

Hence there exists a function B such that

$$b^i = \frac{\partial B}{\partial x_i}\,.$$

In other words

$$b_i = a_{ij}\frac{\partial B}{\partial x_j} \qquad \text{for every } i\,.$$

Thus H is of the form

$$a_{ij}\frac{\partial^2}{\partial x_i \partial x_j} + a_{ij}\frac{\partial B}{\partial x_j}\frac{\partial}{\partial x_i} + c\,,$$

where a_{ij} is a non singular positive or negative definite constant matrix. Since H is symmetric, B is purely imaginary. Let U be the unitary operator defined by

$$Uf = f \exp - \frac{B}{2}\,.$$

Then

$$H' = U^{-1} H U = a_{ij}\frac{\partial^2}{\partial x_i \partial x_j} + v\,,$$

where v is some real valued function. Further H' satisfies (3.1). Hence substituting H' in (3.1) and (3.4) and equating constant terms we get

$$a_{ij}\frac{\partial v}{\partial x_j} = \frac{V_i}{2m_i} \quad \text{for all } i\,.$$

In order that such a v may exist it is necessary and sufficient that

$$A^{-1}M^{-1}J = J'M^{-1}A^{-1}\,,$$

where A, M, J, J' are the matrices described in the statement of the theorem. This completes the proof.

§ 4. Quantum Mechanical Systems on a Riemannian Manifold

Let H be the dynamical operator of a quantum mechanical system whose configuration space is a connected C^∞ Riemannian manifold M of dimension n (the obvious modifications needed for the C^2 manifold can be made by the reader). We shall suppose that H is a second order symmetric differential operator acting in the Hilbert space $L_2(\mu)$ of complex valued functions square integrable with respect to the Riemannian measure μ.

Let U be a fixed coordinate neighbourhood. We shall denote by $L_2(\mu, U)$ and $L_2(U)$ respectively the Hilbert spaces of complex valued functions on U square integrable with respect to the restriction of μ to U and the Lebesgue measure in U. Then there is a canonical isomorphism between $L_2(\mu, U)$ and $L_2(U)$ through a multiplication operator. We shall denote by H_U the restriction of H to U. H_U can be considered as an operator in $L_2(\mu, U)$. The isomorphism between $L_2(\mu, U)$ and $L_2(U)$ takes the operator H_U to an operator H'_U in $L_2(U)$. H'_U is a second order symmetric differential operator in $L_2(U)$.

In the preceding section we derived the form of H under the assumption that the acceleration operators of the individual position coordinates are multiplication operators. In the case of a Riemannian manifold we have to replace the acceleration operators by slightly different ones since the connection coefficients enter the geodesic equations.

Suppose g_{ij} are the coefficients of the Riemannian metric, Γ^k_{ij} the connection coefficients and R^i_{jkl} the components of the curvature tensor derived from the metric in the neighbourhood U. We shall always assume that whenever there is a repeated index in any product expression summation has been carried over it. Any geodesic in U is a solution of the differential equations

$$\ddot{x}_k + \dot{x}_i \Gamma^k_{ij} \dot{x}_j = 0\,, \qquad k = 1, 2, \ldots, n.$$

Hence we shall assume that the operators H'_U satisfy the condition that

$$[H'_U, [H'_U, x_k]] + [H'_U, x_i]\, \Gamma^k_{ij}\, [H'_U, x_j]$$

is a multiplication operator for every k.

Before stating our main result we shall introduce a notation. Consider R_{ijkl} obtained by lowering the index i in the component R^i_{jkl} of the curvature tensor. For the antisymmetric pairs of indices ij ($i < j$) and kl ($k < l$) in R_{ijkl} introduce the labels I and J. Then $((R_{IJ}))$ is a matrix of order $\frac{n(n-1)}{2}$. Let

$$C_U = \det((R_{IJ}))\,.$$

We now have the following theorem.

Theorem 4.1. *Let H be a second order symmetric differential operator in $L_2(\mu)$. Let U be a simply connected coordinate neighbourhood such that $C_U \neq 0$ for every point in U and*

$$H'_U = a_{ij} \frac{\partial^2}{\partial x_i \partial x_j} + b_i \frac{\partial}{\partial x_i} + c$$

where $((a_{ij}))$ is nonsingular in U, a_{ij}, b_i and c are C^∞ functions. Suppose

$$[H'_U, [H'_U, x_k]] + [H'_U, x_i]\, \Gamma^k_{ij}\, [H'_U, x_j] = V_k \text{ for every } k \tag{4.1}$$

where V_k are C^∞ functions. Then H'_U is unitarily equivalent to an operator of the form $h\Delta + V$ in $L_2(\mu, U)$ where Δ is the Laplace-Beltrami operator, h is a constant and V is a C^∞ function. The unitary equivalence can be established through a multiplication operator.

Conversely any operator of the form $h\Delta + V$ as described above always satisfies Eq. (4.1) *if we choose V_k appropriately.*

Remark. In the case when the manifold has dimension 2 the matrix $((R_{IJ}))$ is of order one and C_U is just the Gaussian curvature. The condition of the theorem thus reduces to the manifold possessing non zero curvature at every point in U.

If G is the group of all complex $n \times n$ matrices of determinant one, $n > 2$ and K is the subgroup of unitary matrices then G/K is a symmetric space which is an analytic Riemannian manifold with $C_U \equiv 0$ for every coordinate neighbourhood U.

Proof of Theorem 4.1. The operator $[H'_U, [H'_U, x_i]]$ is of the form given by (3.4). We adopt the same notations as in § 3. An easy calculation shows that

$$[H'_U, x_i]\,\Gamma^t_{ij}\,[H'_U, x_j] = 4\Gamma^t_{ij}\,a_{ik}a_{jl}\frac{\partial^2}{\partial x_k \partial x_l}$$
$$+ \left(4\,a_{ik}\,\Gamma^t_{ij,k}a_{jl}\frac{\partial}{\partial x_l} + a_{ik}\,\Gamma^t_{ij}\,a_{jl,k}\frac{\partial}{\partial x_l}\right) + 4a_{ik}\,\Gamma^t_{ij}\,b_j\frac{\partial}{\partial x_k}$$
$$+ \Gamma^t_{ij}\,b_i b_j + 2a_{ik}\,\Gamma^t_{ij,k}b_j + 2a_{ik}\,\Gamma^t_{ij}\frac{\partial b_j}{\partial x_k} \tag{4.2}$$

where $\Gamma^t_{ij,k}$ denotes $\frac{\partial \Gamma^t_{ij}}{\partial x_k}$. From (3.4), (4.1) and (4.2) we have

$$a_{kr}a_{il,r} - a_{ir}a_{kl,r} + a_{rl}a_{ik,r} + 2\Gamma^i_{rs}a_{rk}a_{sl} = 0 \tag{4.3}$$

for every i, k, l. Interchanging i and k in the above equation and adding to same we obtain

$$a_{sl}\{a_{ik,s} + \Gamma^i_{rs}a_{rk} + \Gamma^k_{rs}a_{ri}\} = 0 \tag{4.4}$$

for every i, k, l. Since $((a_{ij}))$ is non singular in U, (4.4) implies

$$a_{ik,s} + \Gamma^i_{rs}a_{rk} + \Gamma^k_{rs}a_{ri} = 0 \tag{4.5}$$

for every i, k, s. This simply means that the covariant derivative of the second order symmetric tensor with components a_{ij} vanishes identically in U.

The integrability condition for the Eq. (4.5), i.e.,

$$\frac{\partial}{\partial x_t}(\Gamma^i_{rs}a_{rk} + \Gamma^k_{rs}a_{ri}) = \frac{\partial}{\partial x_s}(\Gamma^i_{rt}a_{rk} + \Gamma^k_{rt}a_{ri})$$

can be rewritten as

$$(\tilde{a}_{im}g_{jn} - \tilde{a}_{nj}g_{im})\,R^{nm}{}_{kl} = 0 \tag{4.6}$$

where $\tilde{a}_{ij}$ are the components of the matrix inverse to $((a_{ij}))$. Since $C_U \neq 0$, the matrix $((R_{IJ}))$ is non singular and hence $((R^I_J))$ is non singular. Thus (4.6) holds if and only if

$$\tilde{a}_{ij} = \varrho g_{ij} \qquad \text{for all } i, j$$

where ϱ is a function. Hence $a_{ij} = \varrho^{-1}g^{ij}$. If we substitute g^{ij} for a_{ij}, (4.5) is automatically satisfied. By substituting $\varrho^{-1}g^{ij}$ in (4.5) we obtain $\frac{\partial \varrho^{-1}}{\partial x_s} = 0$ for all s. Thus ϱ^{-1} is a constant. In other words there exists a constant h such that

$$a_{ij} = hg^{ij} \qquad \text{for all } i, j\,. \tag{4.7}$$

Using Eq. (3.4) (with $H = H'_U$), (4.2) and (4.7) and equating the coefficient of $\frac{\partial}{\partial x_u}$ in the left hand side of (4.1) to zero, we get

$$hg^{kl}\frac{\partial^2 g^{tu}}{\partial x_k \partial x_l} + \left(g^{ul}\frac{\partial b_t}{\partial x_l} + b_l\frac{\partial g^{tu}}{\partial x_l} - g^{tl}\frac{\partial b_u}{\partial x_l}\right)$$
$$+ 2h\left(g^{ik}\,\Gamma^t_{ij,k}\,g^{ju} + g^{ik}\,\Gamma^t_{ij}\frac{\partial g^{ju}}{\partial x_k}\right) + 2g^{iu}\,\Gamma^t_{ij}b_j = 0 \tag{4.8}$$

for all t, u. Interchanging t and u in (4.8), adding to the same and making use of (4.5) we obtain simply $0 = 0$.

We shall denote the vector field $g^{ul}\frac{\partial}{\partial x_l}$ by X_u. Interchanging t and u in (4.8) and subtracting from the same we obtain

$$(X_u b_t - X_t b_u) + b_j(g^{ts}X_u g_{js} - g^{us}X_t g_{js}) \\ + hX_j(g^{ts}X_u g_{js} - g^{us}X_t g_{js}) = 0 \quad \text{for every } t, u\,. \tag{4.9}$$

Writing $c_s = b_j g_{js}$ and making use of the standard properties of vector fields, (4.9) can be rewritten as

$$(g^{ts}X_u - g^{us}X_t)\,(c_s + hX_j g_{js}) = 0 \tag{4.10}$$

for all t, u. Multiplying the left hand side of (4.10) by $g_{kt}g_{lu}$ and adding over all t and u, we obtain

$$\frac{\partial}{\partial x_l}(c_k + hX_j g_{jk}) = \frac{\partial}{\partial x_k}(c_l + hX_j g_{jl})$$

for all k and l. Since U is simply connected there exists a C^∞ function d on U such that

$$\frac{\partial d}{\partial x_k} = c_k + hX_j g_{jk} \quad \text{for all } k\,.$$

Hence

$$b_t = g^{ts}c_s = X_t d + h\frac{\partial g^{tr}}{\partial x_r} = X_t d + h\,\mathrm{div}_L X_t\,,$$

where div_L denotes the divergence with respect to the Lebesgue measure. Thus

$$H'_U = h\left(g^{ij}\frac{\partial^2}{\partial x_i\partial x_j} + \mathrm{div}_L X_i\frac{\partial}{\partial x_i}\right) + (X_i d)\frac{\partial}{\partial x_i} + c\,.$$

Since H'_U and $g^{ij}\frac{\partial^2}{\partial x_i\partial x_j} + \mathrm{div}_L X_i\frac{\partial}{\partial x_i}$ are symmetric operators in $L_2(U)$ it follows that d must be purely imaginary. Consider the unitary operator W of $L_2(U)$ into itself defined by

$$Wf = f\exp - \frac{d}{2h}\,.$$

Then

$$W^{-1}H'_U W = h\left(g^{ij}\frac{\partial^2}{\partial x_i\partial x_j} + \mathrm{div}_L X_i\frac{\partial}{\partial x_i}\right) + c'$$

where c' is some function. If this operator is carried over to the space $L_2(\mu, U)$ through the canonical isomorphism it is of the form

$$h\left(g^{ij}\frac{\partial^2}{\partial x_i\partial x_j} + \mathrm{div}_\mu X_i\frac{\partial}{\partial x_i}\right) + V$$

where V is a C^∞ function. Since the Laplace-Beltrami operator is given by the coefficient of h in the above expression this completes the proof of theorem 4.1.

Remark. In general the solution to Eq. (4.5) need not be unique. If however the manifold is analytic and so are the coefficients a_{ij} then a_{ij} are completely determined by (4.5) if we know their values at one point in U. In particular if $a_{ij} = \alpha \cdot g^{ij}$ at any one point in U, then $a_{ij} = \alpha g^{ij}$ at all points in U. Thus the condition that $C_U \neq 0$ at all points in U may be replaced by the analyticity of the manifold M and the coefficients a_{ij} and the equation $a_{ij} = \alpha g^{ij}$ at some point in U.

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