A consistent Lie algebraic representation of quantum phase and number operators

M. Rasetti\#,*

\# Dipartimento di Fisica, Politecnico di Torino, I-10129 Torino, Italy
* Istituto Nazionale di Fisica della Materia, Unità Politecnico di Torino, I-10129 Torino, Italy

A consistent realization of the quantum operators corresponding to the canonically conjugate phase and number variables is proposed, resorting to the $\kappa = \frac{1}{2}$ positive discrete series of the irreducible unitary representation of the Lie algebra $su(1,1)$ of the double covering group of $SO^+(1,2)$.

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The problem – quite relevant both for quantum optics and the physics of mesoscopic systems (Josephson junctions) – of how to represent the canonically conjugate phase $\hat{\phi}$ and number $\hat{n}$ operators $[\hat{\phi}, \hat{n}] = i$ as self-adjoint operators in the Hilbert (e.g. Fock) space $\mathcal{F}$ of states of the corresponding physical system remains essentially unsolved. The several attempts made over the years [1]–[10], have clarified a number of interesting features and have proposed practical approaches to deal with various obstructions, but none has fully overcome the difficulties, inherent essentially to the inconsistency related with the definition of the phase in the state where the number eigenvalue is zero (a difficulty which has a classical counterpart [11]).

The correspondence principle of quantum mechanics appears to suggest that the customary annihilation and creation operators $a, a^\dagger$ (related to the complex classical amplitude of harmonic oscillations) adopted e.g., in the description of the harmonic oscillator, which together with the number $\hat{n}$ and identity operator $\mathbb{1}$, generate the Weyl-Heisenberg algebra $h(1) \left( [a,a^\dagger] = \mathbb{1}, [a,\hat{n}] = a, [a^\dagger,\hat{n}] = -a^\dagger, [\mathbb{1},\mathbb{1}] = 0 \right)$, may be represented in polar form (phase-modulus decomposition) as

$$ a \doteq \hat{\phi} \sqrt{\hat{n}}, \quad (1) $$

$\hat{\phi}$ defining the quantum phase operator. However, it is not possible to derive from the above ansatz a fully satisfactory phase observable: indeed, the solution of (1)

$$ \hat{\phi} = \sum_{n=0}^{\infty} |n\rangle \langle n+1|, \quad \text{where} \ \hat{n} |n\rangle = n |n\rangle, \quad n \geq 0, \quad \text{turns out not to be unitary;} $$

$$ \hat{\phi} \hat{\phi}^\dagger = \mathbb{1}, \ \hat{\phi}^\dagger \hat{\phi} = \mathbb{1} - |0\rangle \langle 0| \ . \quad (2) $$

The approach to the problem most adopted in the applications is that due to Pegg and Barnett [8], who propose to resort to a finite dimensional [12] Hilbert space of of states $\mathcal{H}_N \doteq \text{span}\{|n\rangle | n = 0, \ldots, N - 1 \}$ ($N = \text{dim}(\mathcal{H}_N)$) and to define in it a self adjoint phase operator $\hat{\phi}_N$ by constructing first the set of $N$ phase states

$$ |\phi_\ell\rangle \doteq N^{-\frac{1}{2}} \sum_{n=0}^{N-1} \exp \left( in \phi_\ell \right) |n\rangle, \quad \phi_\ell \doteq \phi_0 + 2\pi \frac{\ell}{N}, \quad (3) $$

for $\ell \in \mathbb{Z}_N$, and setting then $\hat{\phi}_N \doteq \sum_{\ell=0}^{N-1} \phi_\ell |\phi_\ell\rangle \langle \phi_\ell|$. In the occupation number basis $\phi_N$ has matrix elements

$$ \langle \ell | \hat{\phi}_N | \ell \rangle = \phi_0 + \pi \left( N - 1 \right) N^{-1} \quad \text{and, for} \ m \neq \ell, \quad \langle m | \hat{\phi}_N | \ell \rangle = \frac{2\pi^2}{N} \left| \sin \left( \frac{\pi}{N} \left( m - \ell \right) \right) \right|^{-1} e^{i(m-\ell)(\phi_0 + \frac{\pi}{2})} \ . $$

The problem here is that the spectral resolution of the discrete operator $\hat{\phi}_N$ does not provide [13] a measure converging either to a projection valued measure nor to a probability operator measure in the limit $N \to \infty$ (i.e. in the full Hilbert-Fock space $\mathcal{F}$).

The most promising approaches to circumvent such difficulties came from the identification of the algebraic structure underlying the problem. Ref. [14] resorts first to the polar decomposition of step operators in $u(2) \equiv u(1) \otimes su(2)$ and then to its contraction limit. Being $su(2)$ compact, the closure property in this way is lost. At this point the idea of using $su(1,1)$, non-compact counterpart of $su(2)$, was introduced [7], [15], based on relative number variables, well defined (e.g. in the frame of thermo-field dynamics) in a two-mode representation of $su(1,1)$. The crucial notion in these approaches was just the realization of the role of such algebra. This notion was recently revived. Observing that in a canonical quantization scheme the self-adjoint Lie algebra generators $K_1, K_2, K_3$ of the group $SO^+(1,2)$ correspond to the classical polar coordinates variables in $\mathbb{R}^2, R_x = r \cos \phi, R_y = r \sin \phi$ and $R_z = r$, respectively, whose Poisson brackets $\{R_x, R_y\}_{PB} = R_z, \{R_z, R_x\}_{PB} = -R_y, \{R_z, R_y\}_{PB} = R_x$ satisfy the same algebra, Kastur [16] proposed a group theoretical approach to the problem resorting to the irreducible unitary representations of the positive series.

The generators $K_1, K_2, K_3$ have commutation relations $[K_1, K_2] = -iK_3, [K_2, K_3] = iK_1, [K_3, K_1] = iK_2$, or, introducing the skew raising and lowering operators $K_+ \doteq K_1 \pm iK_2$ acting as ladder operators on the eigenvectors of the Cartan operator $K_3$, generator of the compact subgroup $SO(2)$ of $SO^+(1,2), [K_+, K_-] = -2K_3, [K_3, K_\pm] = \pm K_\pm$. 

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The positive discrete series representation of the algebra \( su(1,1) \) of the double covering of \( SO^+(1,2) \) is characterized [17] by the existence of an highest weight vector \( |\kappa,\Omega\rangle \) (invariant, in representation space, under the action of the maximal compact sub-group \( K \sim U(1) \) of \( SU(1,1) \) [18]), annihilated by the lowering operator \( K_+ \). This means that \( K_-|\kappa,\Omega\rangle \) is not a ket in the representation Hilbert space. Upon identifying \( |\kappa,\Omega\rangle \) with the eigenvector \( |\kappa,0\rangle \) of \( K_3 \) the commutation relations give \( K_-|\kappa,0\rangle \equiv 0 \) (see below). The real number \( \kappa \), characterizing the representation, assumes values \( \kappa = \frac{1}{2}, \frac{3}{2}, 2, \ldots \), and is such that the Casimir operator \( C_2 = K_1^2 + K_2^2 - K_3^2 \) has in that representation eigenvalue \( \kappa(1 - \kappa) \). The positive discrete series irreducible unitary representation \( \mathcal{D}^{(+)}_k \), with \( K_1^+ \equiv K_+ \), is spanned by the complete orthonormal set \( \{ |\kappa,n\rangle \mid n \in \mathbb{N} \} \) of eigenstates of \( K_3, K_3^*|\kappa,n\rangle = (n + \kappa)|\kappa,n\rangle \). The ladder operators \( K_+, K_- \) satisfy the equations

\[
K_+|\kappa,n\rangle = \omega_n (n + 1)|\kappa,n + 1\rangle, \\
K_-|\kappa,n\rangle = \omega_{n-1}^{-1}|\kappa,n - 1\rangle,
\]

where \( \omega_n = e^{i\theta_n} \) is a phase. With no loss of generality \( \theta_n \) can be assumed independent on \( n \) \( (\omega_n = e^{i\theta} \equiv \omega, \forall n \in \mathbb{N}) \). The equations above imply

\[
|\kappa,n\rangle = \omega_n^{-1} \frac{1}{n!} K^n_+|\kappa,0\rangle.
\]

(4)

\( \mathcal{D}^{(+)}_k \) has an interesting realization in \( h(1) \): the basis vector \( \{ \frac{1}{h}, n \} \) can be identified with the eigenvector \( |n\rangle \) of \( 3 \) in \( \mathfrak{g} \), and over \( \mathfrak{g} \):

\[
K_+ \equiv \hat{n} \frac{1}{2} a^+, \quad K_- \equiv a \hat{n} \frac{1}{2}, \quad K_3 \equiv \hat{n} + \frac{1}{2}.
\]

There is a connection between this representation of \( su(1,1) \) and the uniform expansion to which (3) reduces for \( \ell = 0 \), which is at the basis of the lack of coverage mentioned above: a uniform superposition of occupation number eigenstates in \( \mathfrak{g} \) can be straightforwardly constructed in \( \mathcal{D}^{(+)}_k \), in view of (4), as [19]

\[
e^{\omega K_+} |\xi,0\rangle = \sum_{n=0}^{\infty} \frac{1}{n!} K^n_+ |\xi,0\rangle, \quad \text{a state which is manifestly not normalizable.}
\]

For analogy with the classical case \( (\cos \phi = r^{-1} R_x, \sin \phi = r^{-1} R_y) \) in [16] the definition is suggested:

\[
\cos \phi \equiv \frac{1}{2} \left\{ K_3^{-1}, K_1 \right\}, \quad \sin \phi \equiv \frac{1}{2} \left\{ K_3^{-1}, K_2 \right\}.
\]

(5)

In the discrete positive series irreducible unitary representation of \( su(1,1) \), this assumption is analytic for generic \( \kappa \), because \( K_3^{-1} \) is well defined in view of the eigenvalue equation of \( K_3 \), but it has the drawback that \( \cos \phi + \sin \phi^2 \) and \( \cos \phi, \sin \phi \), even though both diagonal, are not equal – respectively to \( \tilde{l} \) and \( \Omega \), as they should be. Indeed, they do satisfy such conditions only for large \( n \):

\[
\left( \cos \phi + \sin \phi^2 \right) |\kappa,n\rangle = \frac{1}{8} \left( f^{(\kappa)}_{n+1} + f^{(\kappa)}_n \right) |\kappa,n\rangle, \\
\left( \cos \phi, \sin \phi \right) |\kappa,n\rangle = \frac{1}{8i} \left( f^{(\kappa)}_{n+1} - f^{(\kappa)}_n \right) |\kappa,n\rangle, \quad (6)
\]

where

\[
f^{(\kappa)}_n \equiv [n(n + 2\kappa - 1)]^{\frac{1}{2}} \left( \frac{1}{n + \kappa} + \frac{1}{n + \kappa - 1} \right) \rightarrow 2.
\]

In this note we suggest that the above scheme can be generalized so as to exhibit all the required features for effective phase-angle quantum variables.

The basic step is the generalization of eqs. (5):

\[
\epsilon \equiv \cos \phi \equiv \{ \mathcal{F}(K_3), K_1 \}, \quad \phi \equiv \sin \phi \equiv \{ \mathcal{F}(K_3), K_2 \}, \quad (7)
\]

where \( \mathcal{F} \) is a function – whose existence will be proved in the sequel – meromorphic in the \( \mathcal{D}^{(+)}_k \)-representation, of the form \( \mathcal{F}(K_3) = n^{-1} (1 - |0\rangle \langle 0|) + \Phi(n) \), where \( \Phi(n) \), whose eigenvalues in \( \mathfrak{g} \) will be written in terms of digamma functions, is such that \( \langle 0| \Phi(n) |0\rangle = 0 \). Such choice guarantees that the commutation relations \( \left[ \hat{n}, \cos \phi \right] = -i \sin \phi, \quad \left[ \hat{n}, \sin \phi \right] = i \cos \phi \), are satisfied \( (\hat{n} = K_3 - \frac{1}{2}) \) and \( \mathcal{F} \) may be selected so as to ensure that the two other conditions are satisfied almost everywhere (i.e. in \( \mathfrak{g} \setminus \{0\} \)). The construction \( \mathcal{F} \) in \( \mathcal{D}^{(+)}_k \) in such a way that:

\[
i \cos \phi + \sin \phi^2 = 1, \quad ii) \quad \left[ \cos \phi, \sin \phi \right] = 0, \quad (8)
\]

proceeds as follows. One observes first \( (|n\rangle \equiv |\frac{1}{h}, n\rangle) \) that

\[
\epsilon_+ |n\rangle = \omega L_{n+1} |n+1\rangle + \omega^{-1} L_n |n-1\rangle, \\
\epsilon_- |n\rangle = -i \omega L_{n+1} |n+1\rangle + i \omega^{-1} L_n |n-1\rangle,
\]

where \( L_n \equiv \frac{1}{2} n \left( \mathcal{F} \left( -\frac{1}{2} \right) + \mathcal{F} \left( n + \frac{1}{2} \right) \right) \). Equivalently,

\[
\epsilon_\pm \equiv (\epsilon \pm i \phi) \equiv e^{\pm i\phi}, \quad \epsilon_\pm = \{ \mathcal{F}(K_3), K_\pm \},
\]

satisfy

\[
\epsilon_+ |n\rangle = 2\omega L_{n+1} |n+1\rangle, \quad \epsilon_- |n\rangle = 2\omega^{-1} L_n |n-1\rangle.
\]

From these, for

\[
\mathcal{O} \equiv \frac{1}{4} \epsilon \left[ (1 + \eta) \epsilon + i(1 - \eta) \phi \right] \left[ (1 + \epsilon \eta) \epsilon - i(1 - \epsilon \eta) \phi \right],
\]

where \( \eta \in \{ \pm 1 \}, \quad (O_{1,1} \equiv c^2, O_{1,-1} \equiv s^2, O_{-1,1} \equiv -iac, O_{1,-1} \equiv iac) \), one finds

\[
\mathcal{O}_{\xi,\eta} |n\rangle = \eta \left[ L_n^2 + \xi L_{n+1} \right] |n\rangle
\]

\[
+ \eta (\omega^2 L_{n+1} L_{n+2} |n+2\rangle + \omega^{-2} L_{n-1} L_n |n-2\rangle),
\]

where \( \xi, \eta \in \{ \pm 1 \} \).
whence \((c^2 + s^2) |n\rangle = 2 \left[ \mathcal{L}_n^2 + \mathcal{L}_{n+1}^2 \right] |n\rangle\), and \([c, s] |n\rangle = 2i \left[ \mathcal{L}_{n+1}^2 - \mathcal{L}_n^2 \right] |n\rangle\). The pursued conditions (8) amount then to requiring that \(\mathcal{L}_{n+1}^2 = \mathcal{L}_n^2 = \frac{1}{2}\), for all \(n \geq 1\), namely that the following system of recursion equations is satisfied by \(F(n) = \mathcal{F}(n + \frac{1}{2})\):

\[
(n + 1)F(n + 1) - nF(n - 1) + F(n) = 0 , \tag{9}
\]

\[
F(n) = \frac{1}{n} - F(n - 1) . \tag{10}
\]

Eqs. (10) and (9) are mutually consistent; thus we only need to consider, e.g., (9). Eq. (10) will simply be used to properly continue the result to \(n = 0\). For \(n \geq 1\), recursion equation (9) can be dealt with by the generating function method. One defines first

\[
f(z) = \sum_{n=1}^{\infty} F(n) z^n , \tag{11}
\]

where \(z\) is an undeterminate. Multiplying eq. (9) by \(z^n\) and summing for \(n\) ranging from 1 to \(\infty\), in view of definition (11) one obtains for \(f\) the differential equation

\[
(1 - z^2) \frac{df}{dz} + (1 - z) f(z) - F(1) = 0 . \tag{12}
\]

In view of (10) we select \(F(1) = 1\), so that, as only one integration constant is required, we may set \(F(0) = 0, \Phi(0) = 0\). The solution of (12) is then

\[
f(z) = -(1 + z)^{-1} \ln(1 - z) . \tag{13}
\]

Expanding (13) as a power series in \(z\) one eventually finds

\[
F(n) = (-)^n \sum_{\ell=1}^{n} \frac{(-)^{\ell}}{\ell} , \forall n \geq 1 . \tag{14}
\]

The sum in (14) can be split into even and odd values of \(\ell\), and has different expressions depending on whether \(n\) is even or odd:

\[
F(2m) = \frac{1}{2} \sum_{r=1}^{m} \frac{1}{r} - \sum_{r=0}^{m-1} \frac{1}{2r + 1} , \quad m \geq 1 ,
\]

\[
F(2m + 1) = -\frac{1}{2} \sum_{r=1}^{m} \frac{1}{r} + \sum_{r=0}^{m} \frac{1}{2r + 1} , \quad m \geq 0 .
\]

Recalling now that \([20]\) \(\sum_{\ell=1}^{k} \frac{1}{\ell} = \gamma + \psi(k + 1)\), and

\[
\sum_{\ell=0}^{k-1} \frac{1}{2\ell + 1} = \frac{1}{2}(\gamma + 2 \ln 2 + \psi(k + \frac{1}{2})) ,
\]

where \(\gamma\) is Euler's constant and \(\psi(z)\) the Digamma function, and that \(\frac{1}{2} \psi(k + \frac{1}{2}) = \psi(2k) - \psi(k) - \ln 2\), one obtains - including as well the condition \(F(0) = 0\), and denoting by \([x]\) the largest integer \(\leq x\) -

\[
F(n) = (1 - \delta_{n,0}) \frac{1}{n} + \Theta(n) , \quad \Phi(n) = (-)^n \left[ \psi(\lfloor \frac{1}{2}(n + 1) \rfloor) - \psi(n) \right] . \tag{15}
\]

We may then conclude that the function entering definition (7) \(\mathcal{F}(K_3) = \mathcal{F}(\hat{n})\), does exist and is well defined as operator [21] over the Fock space \(\mathfrak{F}\) for \(n \geq 1\). With this choice, indeed,

\[
\phi_{\pm} |n\rangle = \omega^n |n + 1\rangle , \quad n \geq 0 ; \quad \phi_- |n\rangle = \omega^{-n} |n - 1\rangle , \quad n \geq 1 .
\]

Still what happens in state \(|0\rangle\) has some subtlety which requires further discussion. Explicit calculation using the scheme discussed above shows that while the conditions (8) hold for all \(|n\rangle\) with \(n \geq 1\), one has \((\cos \phi + \sin \phi)^2 |0\rangle = \frac{1}{2} |0\rangle\), \((\cos \phi, \sin \phi) |0\rangle = -\frac{1}{2}i |0\rangle\) and \(\phi_- |0\rangle = 0\). This is the "fossil remain" \(\tilde{n}\) in our representation of the pathology encountered in all other representations and the price paid for making independent on \(n\) the eigenvalues in (6). The action of \(\phi_-\) is badly defined in state \(|0\rangle\); one finds \(\phi, \phi_- = 1 - |0\rangle\langle 0|, \phi_- \phi_- = \tilde{n}\), namely \(\phi_- = |0\rangle\langle 0|\), the same disease as in (2), even though within a much more robust structure, where sine \((s)\) and cosine \((c)\) operators satisfy the desired conditions \(c^2 + s^2 = 1\), \([c, s] = 0\) in \(\tilde{\mathfrak{F}} \setminus |0\rangle\). The message is clear: in state \(|0\rangle\) operator \(\hat{n}\) is sharp; \(\Delta_0(\hat{n}) = \left[|0\rangle\langle 0| - |\tilde{n}\rangle\langle \tilde{n}|\right]^{\frac{1}{2}} = 0\), then \(\Delta_0(\phi)\) can be arbitrarily large. We find \(\Delta_0(c) = \Delta_0(s) = \frac{1}{2}\), which corresponds to the minimum uncertainty condition \(\Delta_0(c) \Delta_0(s) = \frac{1}{2}\) for the commutation relation \([c, s] = 0\) of \(\tilde{n}\).

The new feature here, however, is that (15) can be analytically continued to \(n = -1\), where, in view of the identity \([20]\) \(\psi(1 - z) = \psi(z) + \pi \cot(\pi z)\), one finds \(F(-1) = 0\). Notice that this is not consistent with (10), which however obviously does not hold for \(n = 0\). For \(n = 0\) a more plausible solution to (10) would instead demand

\[
\lim_{n \to 0} nF(n - 1) = 1 . \tag{16}
\]

This leads to an intriguing possible way out of our difficulty, that consists in replacing \(\Phi(n)\) in (15),

\[
\Phi(n) = (-)^n \left[ \psi(\lfloor \frac{1}{2}(n + 1) \rfloor) - \psi(n) - 2 \delta_{n,1} \psi(n + 1) \right. \\
\left. + \delta_{n,2} \left( \psi(n + 2) - \psi(n + 1) \right) \right] \tag{17}
\]

Indeed, with this new self-adjoint operator \(\hat{n}\), \(\Phi(\hat{n})\), as given by the first of eqs. (15), leads to \(\phi_+ \phi_- = \mathbb{I}\), \(\phi_- \phi_- = 0\) also in state \(|0\rangle\).

There is a price to be paid, of course. What the above construction requires is a non trivial mathematical structure, implying the extension of the space of states \(\tilde{\mathfrak{F}}\) to include an extra vector \(|1\rangle\) \((\{1\} = \mathcal{F}(K_3)K_0|\{0\}\rangle\) which is annihilated by \(K_-\) (it is this requirement that originates the second line in (17)), is actually out of \(\tilde{\mathfrak{F}}\), but out of which \(|0\rangle\) can be generated by \(K_+\). Ket \(-|\rangle\) has the property that \((-|1\rangle - |1\rangle = 1\), and \(\langle n | - 1\rangle = 0\), \(\forall n \geq 0\), leading to the existence of both a \(PVM\) and
a POM in $\mathcal{F}$. The construction of the completed space $\mathfrak{F} \cup \{ -1 \}$ can be consistently and rigorously carried over resorting to the notion of "diluted extension Hilbert space" [23]. The spectral theory for self-adjoint operators shows indeed that one may generally restrict the attention to bounded operators by the use of Cayley transform: if the operator is only symmetric, possibly with dense domain, but not self-adjoint, then the Cayley transform reduces the problem to the analysis of partial isometries. But if the index is non-zero (i.e. the co-dimension of the initial and the final space are unequal) then there will not be self-adjoint extensions in the same, given, Hilbert space, but a dilated extension Hilbert space is needed for a complete understanding of spectral resolutions and self-adjoint operator extensions of unbounded operators. It should be noted that this theory, holds for Lie algebras only in the case they are simple, and requires passing to the universal enveloping algebra to get the appropriate $\ast$-representation.

From the operational point of view, as in our case co-dimension 1 is sufficient, a plausible way to perform the extension is to recall that the principal continuous series of class I and the supplementary series have representations spanned by a basis $\{ \{ \lambda, \mu \} \}$, corresponding to $C_2 = |\lambda|^2 + \frac{i}{2}$, for which $\lambda$ is respectively a nonnegative real number and a pure imaginary $\lambda = i\tau$, $\frac{1}{2} < \tau < \frac{1}{2}$, such that

$$K_{3}^{\mu} |\lambda, \mu \rangle = | \lambda, \mu \rangle \cdot \mu = 0, \pm 1, \pm 2, \ldots, K_{\pm}^{\mu} \mu, \mu \rangle = (\pm (\lambda + i\mu) \pm \mu) | \lambda, \mu \pm 1 \rangle \ .$$

Eqs. (18) imply for $\lambda(\tau) \to 0$, where the two representations are isomorphic with each other and with the discrete series (positive $\cup$ negative, through the identification $K_{\pm}^{\mu} \mu, \mu \rangle \equiv |0, \mu \rangle$ is given, $\forall \mu \geq 1$, by [24]

$$| \mu \rangle = \frac{1}{\mu!} K_{-}^{\mu} |0 \rangle \text{, but } -\mu \rangle = (-\mu)^{1/2} \mu! K_{-}^{\mu} |0 \rangle \ .$$

In other words, the eigenstates are generated by powers of both $K_{+}$ and $K_{-}$. What the desired Hilbert space extension amounts to is including in the discrete positive series $| -1 \rangle$ from one of the two continuous series.

Physically we suggest the interpretation that whereas $|0\rangle$, even though representing a physical "vacuum", namely a state with no excitations (zero occupation number), yet is still in the space of states of the system, $| -1 \rangle$ does instead describe the true vacuum, i.e. emptiness of the state space of the system, out of whose quantum fluctuations such states (in particular $|0\rangle$) can be generated.

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$$\psi \equiv \frac{e^{-x} - e^{-y}}{1 - e^{-x}} \ .$$

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