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Subtle inconsistencies in the straightforward definition of the logarithmic function of annihilation and creation operators and a way to avoid them

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Abstract
Using the resolution of identity spanned by coherent states of the harmonic oscillator, any entire function of the creation and the annihilation operators and its action on a vector in Hilbert space can be defined directly and simply. We show that such a direct approach applied to non-entire functions $\ln\hat{a}$ and $\ln\hat{a}^{\dagger}$, present in the literature, may lead to errors and contradictions. We elucidate their roots and propose a way to avoid them. We discuss the obtained results.

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1. Introduction

Spectral theorem generalizes the representation of the self-adjoint operator in terms of the complete orthonormal system of eigenvectors to include the continuous spectrum. Such a possibility is obtained by introducing the concept of a resolution of the identity, a nondecreasing family $\hat{E}_\lambda$ of projection operators that interpolates between $\hat{0}$ for $\lambda \to -\infty$ and $\hat{I}$ for $\lambda \to \infty$. Spectral theorem guarantees that for every self-adjoint operator $\hat{A}$ there is a unique resolution of identity in terms of which $\hat{A}$ can be expressed as

$$\hat{A} = \int \lambda \, \mathrm{d}\hat{E}_\lambda. \tag{1}$$

The spectral theorem together with functional calculus rules allow one to define the function of the operator $\hat{A}$ in the form

$$f(\hat{A}) = \int f(\lambda) \, \mathrm{d}\hat{E}_\lambda. \tag{2}$$

The annihilation operator of the harmonic oscillator is a non-Hermitian operator. Its eigenstates are coherent states $|\alpha\rangle$ which form an overcomplete and non-orthogonal set, which spans the resolution of identity. In formal analogy with the spectral theorem one can write

$$f(\hat{a}) = \frac{1}{\pi}\int f(\alpha)|\alpha\rangle\langle\alpha|\,\mathrm{d}^2\alpha. \tag{3}$$

It can be checked easily that, when f is an entire function, this representation is correct and consistent in a sense that

$$f(\hat{a})|\alpha_0\rangle = f(\alpha_0)|\alpha_0\rangle = \frac{1}{\pi}\int f(\alpha)|\alpha\rangle\langle\alpha|\alpha_0\rangle\,\mathrm{d}^2\alpha. \tag{4}$$

In the spectral theorem for Hermitian operators no special requirements about the function f were needed for validity of the representation (2). It seems that, by analogy, the representation (3) was uncritically overtaken for the definition of the logarithmic function of $\hat{a}$ so that this function was defined in the literature as [1–3]

$$\ln\hat{a} = \frac{1}{\pi}\int \ln\alpha|\alpha\rangle\langle\alpha|\,\mathrm{d}^2\alpha, \tag{5}$$

with an implicit or explicit assumption that at the same time

$$\ln\hat{a}|\alpha\rangle = \ln\alpha|\alpha\rangle, \qquad \forall\,\alpha. \tag{6}$$

So in [1], as an operator of phase, the operator

$$\hat{\varphi} = \frac{1}{2i}(\ln\hat{a} - \ln\hat{a}^\dagger) \tag{7}$$

was proposed and its matrix elements expressed in the coherent states basis assuming that $\forall\,\alpha\,\ln\hat{a}|\alpha\rangle = \ln\alpha|\alpha\rangle$ and $\langle\alpha|\ln\hat{a}^\dagger = \langle\alpha|\ln\alpha^*$. Some results of [1] were contested in [2]. Using the resolution of unity $\hat{I} = \frac{1}{\pi}\int|\alpha\rangle\langle\alpha|\,\mathrm{d}^2\alpha$ the authors of [2] claimed that the operator $\hat{\varphi}$ may be represented in the form

$$\hat{\varphi} = (2\pi i)^{-1}\int \ln(\alpha/\alpha^*)|\alpha\rangle\langle\alpha|\,\mathrm{d}^2\alpha \tag{8}$$

and identified the last operator with an operator already well known in the literature [4]. We feel that some steps in arguments of the two disputing sides may contain subtle errors. Namely, unlike (3) and (4), conditions (5) and (6) define different operators simply because

$$\ln\hat{a}|\alpha\rangle = \ln\alpha|\alpha\rangle \neq \frac{1}{\pi}\int \ln\alpha'|\alpha'\rangle\langle\alpha'|\alpha\rangle\,\mathrm{d}^2\alpha', \tag{9}$$

as it will be shown in the next section. Due to this, conditions (5) and (6), when assumed to represent the same operator, are inconsistent and may lead to errors when used together and in the same context. We will also prove in the same section that if one accepts by definition that $\ln\hat{a}|\alpha\rangle = \ln\alpha|\alpha\rangle\,\forall\,\alpha$, and this definition may be considered as a correct definition, then $(\ln\hat{a})^\dagger$ is not defined on any $|\alpha\rangle$ so that in this case the domain of definition of the operator formally defined in (7), strictly speaking, is empty.

It seems that both of the mentioned disputed sides were unaware of these facts related to the operators $\ln\hat{a}$ and $\ln\hat{a}^\dagger$. We believe that these questions, especially in respect to the problem of the phase operator, deserve appropriate attention. In section 3 using and adapting the results of Perelomov [5] we show that on the discrete set $|\alpha_i\rangle$ defined on the von Neumann lattice from which, to avoid overcompleteness, one vector must be excluded; the domains of definition for both $\ln\hat{a}$ and $(\ln\hat{a})^\dagger$ coincide, and that this set is a maximal set of coherent states with such a property. We also define the phase operator $\hat{\varphi} = \frac{1}{2\mathrm{i}}(\ln\hat{a} - \ln\hat{a}^\dagger)$ with the von Neumann lattice from which the vector $|0\rangle$ is excluded, as its natural domain of definition, and analyze its main characteristics. In the last section we discuss the obtained results.

2. Some consequences of a definition $\ln\hat{a}|\alpha\rangle = \ln\alpha|\alpha\rangle, \forall\alpha$

As already mentioned, the operators defined by equalities (5) and (6) are different operators. To prove this, let us suppose the opposite, namely that

$$\ln\alpha_0|\alpha_0\rangle = \frac{1}{\pi}\int \ln\alpha|\alpha\rangle\langle\alpha|\alpha_0\rangle\,\mathrm{d}^2\alpha. \tag{10}$$

After the scalar multiplication by $\langle\alpha_0|$ we would have

$$\ln\alpha_0 = \frac{1}{\pi}\int \ln\alpha\langle\alpha_0|\alpha\rangle\langle\alpha|\alpha_0\rangle\,\mathrm{d}^2\alpha. \tag{11}$$

In the general case this equality is not valid. For example if we take a cut in the complex plane along the negative x-axis, denoting by ϑ the phase of the complex number α, we would have $\vartheta \in [-\pi, \pi)$. Taking $\alpha_0 = \mathrm{e}^{-\mathrm{i}\pi}$ we would have $\ln\alpha_0 = -\mathrm{i}\pi$ while on the right-hand side apart from some real constant one would get for the imaginary part

$$\frac{1}{\pi}\int_0^\infty\int_{-\pi}^{+\pi}\vartheta|\langle\alpha_0|\alpha\rangle|^2\,\mathrm{d}\vartheta\,\varrho\,\mathrm{d}\varrho, \tag{12}$$

which is obviously zero. This terminates the proof.

At first sight the obtained result seems a bit paradoxical. Namely, one is accustomed to interchange operators and sign of integration, so that one may uncritically accept as natural the equality

$$\ln\hat{a} = \ln\hat{a}\frac{1}{\pi}\int|\alpha\rangle\langle\alpha|\,\mathrm{d}^2\alpha = \frac{1}{\pi}\int\ln\alpha|\alpha\rangle\langle\alpha|\,\mathrm{d}^2\alpha. \tag{13}$$

However, the operator $\ln\hat{a}$ defined according to (6) is discontinuous on coherent states which approach the cut, so that it is not surprising that one cannot interchange its place with the integration sign. The operators which are the entire functions of the operator $\hat{a}$ are continuous on every $|\alpha\rangle$ and due to this such an interchange for them is allowed.

In respect to possible applications there is still a more serious drawback in the definition of the operator $\ln\hat{a}$ in a way that $\ln\hat{a}|\alpha\rangle = \ln\alpha|\alpha\rangle, \forall\,\alpha$. Namely, physically more interesting is the combination of operators $\ln\hat{a} - \ln\hat{a}^\dagger$, which may be considered as a candidate for a phase operator of the harmonic oscillator, in an analogy to the phase (argument) of the ordinary complex number. We shall now prove that if we define $\ln\hat{a}|\alpha\rangle = \ln\alpha|\alpha\rangle\forall\,\alpha$, then there exists none $|\alpha\rangle$ on which $(\ln\hat{a})^\dagger$ is defined.

Proof. Suppose that at least one $|\alpha_1\rangle$ exists, on which $f(\hat{a}^\dagger)$ is defined so that $f(\hat{a}^\dagger)|\alpha_1\rangle = |\psi_{\alpha_1}\rangle \in L_2$. By definition of the adjoint operator we would have the following relation

$$(|\alpha\rangle, f(\hat{a}^\dagger)|\alpha_1\rangle) \stackrel{\mathrm{def}}{=} (f(\hat{a})|\alpha\rangle, |\alpha_1\rangle) \tag{14}$$

where by (,) we denote the scalar product of vectors $|\alpha\rangle$ in Hilbert space. The right-hand side of this equality gives

$$f^*(\alpha)\langle\alpha|\alpha_1\rangle = f^*(\alpha)\,\mathrm{e}^{-\frac{|\alpha|^2}{2}-\frac{|\alpha_1|^2}{2}+\alpha^*\alpha_1}. \tag{15}$$

The left-hand side of (14) equals

$$(|\alpha\rangle, f(\hat{a}^\dagger)|\alpha_1\rangle) = (|\alpha\rangle, |\psi_{\alpha_1}\rangle) = \langle\alpha|\psi_{\alpha_1}\rangle. \tag{16}$$

Writing $|\psi_{\alpha_1}\rangle = \sum_n c_n|n\rangle$, we can write

$$\langle\alpha|\psi_{\alpha_1}\rangle = \mathrm{e}^{-\frac{|\alpha|^2}{2}}\sum_n\frac{c_n}{\sqrt{n!}}\alpha^{*n}. \tag{17}$$

Since (15) and (17) should be equal, it would follow that

$$f^*(\alpha) = \mathrm{e}^{\frac{|\alpha_1|^2}{2} - \alpha^*\alpha_1} \sum_n \frac{c_n}{\sqrt{n!}} \alpha^{*n}. \tag{18}$$

This equality could be satisfied if and only if $f(\alpha)$ were an entire function. No other class of functions can satisfy such an equality. Since $\ln \alpha$ is not an entire function this terminates the proof. Evidently, the analogous result applies also to the other nonentire functions. □

This result shows that the definition $\ln \hat{a}|\alpha\rangle = \ln \alpha|\alpha\rangle, \forall\, \alpha$, although formally correct, is useless in all situations in which $\ln \hat{a}$ and $(\ln \hat{a})^\dagger$ come together, as is the case for a phase operator (7). The root of this difficulty is the overcompleteness of the set of coherent states $|\alpha\rangle$. To avoid it, the domain of definitions of $\ln \hat{a}$ must be restricted to a discrete set of coherent states $|\alpha_i\rangle$, which is complete but not overcomplete. One way to achieve this is given in the next section.

3. A maximal set of $|\alpha_i\rangle$ on which both $\ln \hat{a}$, $(\ln \hat{a})^\dagger$ and a phase operator $\hat{\varphi} = \frac{1}{2\mathrm{i}}(\ln \hat{a} - (\ln \hat{a})^\dagger)$ may be defined

A discrete subset of coherent states was for the first time introduced by von Neumann 1932 [6], by partitioning of phase space in rectangular cells of the size of the Planck constant h and taking from each cell a single coherent state. He used this construction in order to obtain quantum mechanical operators for most accurate simultaneous unsharp measurements of coordinate and momentum allowed by quantum mechanical laws [4, 7]. Without proof, von Neumann claimed that it was easy to see that the set $|\alpha_i\rangle$ so obtained is complete but not overcomplete. von Neumann's claim about completeness, considered as obvious by himself, was for the first time rigorously proved almost 40 years later by Perelomov [5], who was obliged to consider many related mathematical subtleties. His final results, which will be needed for our further analysis, are the following.

Consider two complex numbers ω_1 and ω_2 which in complex plane represent sides of a parallelogram with an area S. Then the system of coherent states

$$|\alpha_{kl}\rangle = |k\omega_1 + l\omega_2\rangle, \tag{19}$$

where k and l are integers, depending of the value of S, fulfil the following conditions

(a) If $S < \pi$, the system $|\alpha_{kl}\rangle$ is overcomplete.
(b) If $S > \pi$, the system is incomplete.
(c) If $S = \pi$, after exclusion of the one, and only one whichever vector from the system, the system becomes complete.

For the discretized set $\{|\alpha_{kl}\rangle\}$ there exists a biorthogonal set $\{|w_{kl}\rangle\}$ with properties:

$$\langle w_{kl}|\alpha_{k'l'}\rangle = \delta_{kk'}\delta_{ll'} \tag{20}$$

and

$$\hat{I} = \sum_{kl} |w_{kl}\rangle\langle\alpha_{kl}| = \sum_{kl} |\alpha_{kl}\rangle\langle w_{kl}|. \tag{21}$$

This biorthogonal set is unique. Namely, if another biorthogonal set $\{|w'_{kl}\rangle\}$ existed, then the scalar product of the difference of corresponding vectors from the two sets, $|w'_{kl}\rangle - |w_{kl}\rangle$, with every vector from the set $\{\alpha_{kl}\rangle\}$ would be equal to zero. This fact, together with the fact that the set $\{|\alpha_{kl}\rangle\}$ is complete, implies that $|w'_{kl}\rangle = |w_{kl}\rangle$. In our considerations we found convenient to choose the square elementary cell so that we have

$$|\alpha_{kl}\rangle = |\sqrt{\pi}(k - \mathrm{i}l)\rangle. \tag{22}$$

We excluded the vector $|\alpha = 0\rangle$ since the logarithmic function is not defined there.

Now using this discretized resolution of unity, we can define

$$\ln \hat{a} = \sum_{kl} \ln \alpha_{kl} |\alpha_{kl}\rangle\langle w_{kl}| \quad (\ln \hat{a})^\dagger = \sum_{kl} \ln \alpha^*_{kl} |w_{kl}\rangle\langle \alpha_{kl}|. \tag{23}$$

It is obvious that both $\ln \hat{a}$ and $(\ln \hat{a})^\dagger$ are defined on the same set of coherent states $|\alpha_{kl}\rangle$ and that with these definitions all the above analyzed difficulties are avoided. We also see that $(\ln \hat{a})^\dagger = \ln \hat{a}^\dagger$. For a phase operator $\hat{\varphi} = \frac{1}{2\mathrm{i}}(\ln \hat{a} - (\ln \hat{a})^\dagger)$ we have now a domain of definition $|\alpha_{kl}\rangle$ which is a complete set, and we can write

$$\hat{\varphi} = \frac{1}{2\mathrm{i}} \sum_{kl} (\ln \alpha_{kl} |\alpha_{kl}\rangle\langle w_{kl}| - \ln \alpha^*_{kl} |w_{kl}\rangle\langle \alpha_{kl}|). \tag{24}$$

Every candidate for a phase operator to be physically acceptable, must fulfil at least the two following conditions: (i) The average value for this operator in coherent states $|r\,\mathrm{e}^{\mathrm{i}\Theta}\rangle$ for high r should approach Θ. (ii) For states $|n\rangle$ the phase should be distributed completely randomly, so that accepting $\vartheta \in [-\pi, \pi)$ the average value $\langle n|\hat{\varphi}|n\rangle$ should be equal to zero. Condition (i) for coherent states $\{|\alpha_{kl}\rangle\}$ is fulfilled exactly. For the other coherent states, as our preliminary numerical results show [8], $\langle \alpha|\hat{\varphi}|\alpha\rangle$ differs from $\arg \alpha$ for a couple percents. Condition (ii) is fulfilled exactly, as we will now show.

First, we have

$$\langle n|\hat{\varphi}|n\rangle = \frac{1}{2\mathrm{i}} \sum_{kl} \langle n| \big[\ln \alpha_{kl} |\alpha_{kl}\rangle\langle w_{kl}| - \ln \alpha^*_{kl} |w_{kl}\rangle\langle \alpha_{kl}| \big] |n\rangle. \tag{25}$$

We choose $\omega_1 = \sqrt{\pi}, \quad \omega_2 = -\mathrm{i}\sqrt{\pi}$ so that $\alpha_{k,-l} = \alpha^*_{k,l}$. We have

$$\langle n|\alpha_{kl}\rangle\langle w_{kl}|n\rangle = \frac{1}{\pi} \int \mathrm{d}^2\alpha \langle n|\alpha_{kl}\rangle\langle w_{kl}|\alpha\rangle\langle \alpha|n\rangle = A_{kl}. \tag{26}$$

Introducing the notations $\beta_{mn} = m\omega_1^* + n\omega_2^*$, $\alpha_{kl} = k\omega_1 + l\omega_2\, \alpha^*_{kl} = \beta_{kl}$ and the function

$$\sigma(\alpha) = \alpha \prod_{m,n} \left(1 - \frac{\alpha}{\beta_{mn}}\right) \mathrm{e}^{\frac{\alpha}{\beta_{mn}} + \frac{1}{2}\left(\frac{\alpha}{\beta_{mn}}\right)^2}, \tag{27}$$

according to the results of Perelomov [5] we have

$$\langle \alpha|w_{kl}\rangle = (-1)^{k+l+kl}\, \mathrm{e}^{-\frac{|\alpha|^2}{2}} \alpha^*_{kl} \frac{\sigma(\alpha^*)}{\alpha^*(\alpha^* - \alpha^*_{kl})}, \tag{28}$$

It is straightforward to verify that

$$A_{k,l} = A^*_{k,-l}. \tag{29}$$

The first part of the sum in (25), the one with $\ln \alpha_{kl}$, can be split into sum of conjugate pairs $\ln \alpha_{kl} A_{kl} + \ln \alpha_{k,-l} A_{k,-l}$. Each of them is a real number $2\mathrm{Re}(\ln \alpha_{kl} A_{kl})$. The other part of the sum, the one with $\ln \alpha^*_{kl}$ is conjugate to the first, i.e. it is the same real number. Therefore subtraction in (25) gives zero as a result.

4. Conclusions and discussion

From our results we can conclude that

(1) Starting from coherent states as a domain of definition for $\ln \hat{a}$ and $\ln \hat{a}^\dagger$, in order to obtain a common domain for both these operators, one must restrict the domain of definition to a discrete set of coherent states which is complete but not overcomplete.

(2) The results of Perelomov show that the partitioning of the α-plane in congruent parallelogram cells with the area equal to π—what in the phase space corresponds to the Planck constant h—choosing a single coherent state from each but whichever one cell, one obtains a complete set. Excluding the vector $|0\rangle$ one obtains a natural domain of definition for the phase operator $\hat{\varphi} = \frac{1}{2i}(\ln \hat{a} - \ln \hat{a}^\dagger)$.

(3) We are not aware of any analogous result, which would guarantee for some other set $|\alpha_i\rangle$ that it is complete but not overcomplete.

(4) We used square cells to make calculations simpler, which even in this geometrically simplest case are very complicated. For different choice of cells one would get a different domain of definition and consequently a different phase operator $\hat{\varphi}$. However, these operators would not differ qualitatively and even quantitatively, as our numerical results for coherent states show [8], would be close to each other.

(5) The operator $\frac{1}{2\pi \mathrm{i}} \int \mathrm{d}^2\alpha \ln(\alpha/\alpha^*)|\alpha\rangle\langle\alpha|$, having very interesting physical features [9], although in this form correctly defined, can in no rigorous sense be considered to represent the operator function $\frac{1}{2\mathrm{i}}(\ln \hat{a} - \ln \hat{a}^\dagger)$.

Various approaches to the 'quantum phase' have been proposed but different approaches give predictions, which differ not only quantitatively but also even qualitatively. In this sense the question 'what quantum phase really is' does not have a generally accepted answer [10]. In a very rich and insightful paper [11] it was argued that as 'phase' is an essentially classical notion, and a classical phase can be assigned unambiguously to a quantum state only if in phase space it may be represented as a large amplitude localized state, infinitely many different Hermitian operators qualify as 'phase operators'. They only have to describe the phase in such a case correctly, and all are expressible as

$$\hat{\Phi} = [\tan^{-1}(\hat{p}/\hat{q})]_\Omega, \tag{30}$$

where Ω specified an ordering rule [11]. The 'canonical' ordering is Weyl ordering [12, 13]. Although our operator defined by equations (24), for the first time announced in [14], satisfies the condition regarding the phase of the mentioned states, it is not of the form (30), and the problem of phase ordering does not arise in it. As it fulfils physical conditions for the mean value of phase for states for which this value is evident *a priori*, and represents the closest correct operator analogon of the argument (phase) of the ordinary complex number, it may be considered as a one more reasonable candidate for the phase operator. It also may be expected that its further investigation may contribute to some elucidation of the 'quantum phase problem' in an analogous way as in various respects did all the other phase operators introduced so far.

Finally, a couple of remarks of the mathematical character. The operators $\ln \hat{a}$ and $(\ln \hat{a})^\dagger$, as defined in equation (23), have some 'family resemblance' with their originators $\hat{a}$ and $\hat{a}^\dagger$, but also some different and at the first sight unexpected features. So, $\ln \hat{a}$ inherits in a sense the property of $\hat{a}$, to have as its eigenvectors all coherent states on which it is defined, namely the coherent states on the lattice $|\alpha_{\mathrm{i}k}\rangle$. On the other hand the operator $\hat{a}^\dagger$ has no eigenvectors. However, all the vectors of the biorthogonal set $\{|w_{\mathrm{i}k}\rangle\}$ are the eigenvectors of the operator $(\ln a)^\dagger$, as it is evident from the orthogonality relation (20), and definition (23). This new feature is a direct consequence of the new discrete domain of definition of this operator and the existence of the corresponding biorthogonal set $\{|w_{\mathrm{i}k}\rangle\}$.

All our mathematical considerations in this work were on a somewhat intuitive physical level of rigor. It would be desirable to have a mathematically more rigorous foundation of the introduced operators. We feel, by historical analogy with rigorous mathematical foundation of the celebrated von Neumann lattice, that such results are not at hand.

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