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## LETTER TO THE EDITOR

## Note on canonical quantization and unitary equivalence in field theory

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### Abstract

The problem of defining and constructing representations of the canonical commutation relations can be systematically approached via the technique of *algebraic quantization*. In particular, when the phase space of the system is linear and finite dimensional, the ‘vertical polarization’ provides an unambiguous quantization. For infinite-dimensional field theory systems, where the Stone–von Neumann theorem fails to be valid, even the simplest representation, the Schrödinger functional picture has some non-trivial subtleties. In this letter we consider the quantization of a real free scalar field—where the Fock quantization is well understood—on an arbitrary background and show that the representation from the most natural application of the algebraic quantization approach is not, in general, unitarily equivalent to the corresponding Schrödinger–Fock quantization. We comment on the possible implications of this result for field quantization.

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### 1. Introduction

The process of constructing a quantum theory starting from a given classical system is not by any means a simple *recipe procedure*. Indeed, the quantization process is full of choices that might lead to inequivalent quantum theories. This ambiguity in the quantization process is a well-known fact, for instance, when trying to define operators for quadratic momentum observables due to factor ordering issues. In this letter we shall focus our attention on canonical quantization methods; that is, we will start by considering a phase space  $\Gamma$  which, for simplicity, can be linear with coordinates  $(q^i, p_j)$ . The final goal is to have a quantum system described by a Hilbert space  $\mathcal{H}$  and a set of (Hermitian) operators  $\hat{O}_j$  associated with real observables. In the past few decades, a manifold of methods to deal with these problems has appeared with

varying success. In very broad terms, they differ on the basic objects/properties of the classical system that is used to perform the quantization process. For instance, the *group theoretical* quantization places special attention on the symmetry group of the classical phase space [1]; the geometric quantization programme tries to describe the process in terms of sections of bundles on phase space [2], etc. Of particular relevance is the programme known as the *algebraic quantization method*, pioneered by Ashtekar [3] and its refined version (all tailored to deal with constrained systems) known as refined algebraic quantization [4]. The basic idea of this programme is to identify a suitable algebra of observables on phase space for which there will be unambiguous operators satisfying the canonical commutation relations (CCR). The programme also involves the choice of vector space  $V$  where the quantum operators  $\hat{O}_i$  are defined, and an inner product on  $V$  that makes the operators have the desired *reality conditions*. This constitutes the ‘kinematical’ part of the quantization. Dynamical issues, such as implementation of the Hamiltonian or quantum constraints, are generally regarded as a second step in the process.

When the system is finite dimensional the quantization process has a preferred endpoint in the well-known Schrödinger representation, which in the geometric quantization language represents the *vertical polarization* (wavefunctions depend only on the configuration space variables  $q^i$ ). For alternative ‘polymer’ representations where the configuration observable is not well defined, see [5]. The Stone–von Neumann theorem assures us that any ‘decent’ representation will be unitarily equivalent to the usual Schrödinger one.

In the case of a field theory system with an infinite number of degrees of freedom, it is known that the CCR accept infinite non-equivalent representations (for a very readable discussion on this issue, see [6]). This feature of field theory has an important consequence in the definition of the QFT on curved spacetimes where different observables might disagree on the observable predictions of the theory. In the case of Fock representations, the relevant construct in the quantization process responsible for this ambiguity is well understood in terms of Bogoliubov transformations. Although several attempts have been made to understand the subtleties of Schrödinger representations [7, 8], a systematic construction for general curved spacetimes has only been considered recently [9]. It is important then to explore and understand the various objects involved in the quantization process and its relation to the existence of (in-)equivalent quantum representations. The purpose of this letter is to explore these issues and analyse the algebraic quantization programme in view of the existing canonical quantization of the scalar field as done in [9]. That is, we shall follow the algebraic construction, using the most natural choices along the way, and compare the resulting quantization with [9].

The structure of the letter is as follows. In section 2, we recall the algebraic quantization programme in general and then consider the case of the free real scalar field using this prescription. In section 3, we consider the quantization of the scalar field, following the algebraic approach and then compare this picture with the representation from a different viewpoint [9]. In section 4 we study the origin of this discrepancy and recall the unitary implementation of linear canonical transformation in quantum mechanics. We find that even when, naively, the two representations are unitarily equivalent (as is the case in finite-dimensional systems), the required transformation does not exist; the two representations are, in general, non-unitary. We conclude in section 5 with a discussion of the results.

## 2. Preliminaries

This section has two parts. In the first, we recall basic features about algebraic quantization and in the second, we review the case of a real scalar field.

### 2.1. Algebraic quantization: general formalism

A physical system in the canonical perspective is normally represented, at the classical level, by a *phase space*  $\Gamma$ , endowed with a symplectic structure  $\Omega$ . The phase space is denoted by  $(\Gamma, \Omega)$ . The Lie algebra of vector fields on  $\Gamma$  induces a Lie algebra structure on the space of functions, given by  $\{f, g\} := -\Omega_{ab}X_f^aX_g^b = \Omega^{ab}\nabla_a f\nabla_b g$  such that  $X_{\{f,g\}}^a = -[X_f, X_g]^a$ . The ‘product’  $\{\cdot, \cdot\}$  is called a *Poisson bracket* (PB).

In very broad terms, by quantization one means the passage from a classical system, as described in the last part, to a quantum system. Observables on  $\Gamma$  are to be promoted to self-adjoint operators on a Hilbert space. However, we know that not all observables can be promoted unambiguously to quantum operators satisfying the CCR. A well-known example of such a problem is factor ordering. What we *can* do is to construct a subset  $\mathcal{S}$  of *elementary classical variables* for which the quantization process has no ambiguity. This set  $\mathcal{S}$  should satisfy the following two properties.

1. The set  $\mathcal{S}$  should be a vector space large enough so that every (regular) function on  $\Gamma$  can be obtained by (possibly a limit of) sums of products of elements in  $\mathcal{S}$ . The reason for this condition is that we want enough observables to be unambiguously quantized.
2. The set  $\mathcal{S}$  should be small enough such that it is closed under Poisson brackets.

The next step is to construct an (abstract) quantum algebra  $\mathcal{A}$  of observables from the vector space  $\mathcal{S}$  as the free associative algebra generated by  $\mathcal{S}$  (for a definition and discussion of free associative algebras see [11]). It is in this quantum algebra  $\mathcal{A}$  that we impose the Dirac quantization condition: given  $A, B$  and  $\{A, B\}$  in  $\mathcal{S}$  we impose

$$[\hat{A}, \hat{B}] = i\hbar\widehat{\{A, B\}}. \quad (1)$$

It is important to note that there is no factor order ambiguity in the Dirac condition since  $A, B$  and  $\{A, B\}$  are contained in  $\mathcal{S}$  and they have associated a unique element of  $\mathcal{A}$ .

The next step is to find a vector space  $V$  and a representation of the elements of  $\mathcal{A}$  as operators on  $V$ . The reality conditions (encoded as  $*$ -relations on  $\mathcal{A}$ ) are used as a criterion for finding the inner product  $\langle \cdot, \cdot \rangle$  on  $V$  that transforms these relations into Hermiticity conditions. That is, real observables on  $\mathcal{S}$  should become Hermitian operators on  $V$ . Finally, one completes  $V$  to get the Hilbert space  $\mathcal{H}$  of the theory. For details of this approach to quantization, see [3].

In the case where the phase space  $\Gamma$  is a linear space, there is a particularly simple choice for the set  $\mathcal{S}$ . We can take a global chart on  $\Gamma$  and choose  $\mathcal{S}$  to be the vector space generated by *linear* functions on  $\Gamma$ . In some sense this is the smallest choice of  $\mathcal{S}$  one can take. We can now look at these linear functions on  $\Gamma$ . Denote by  $Y^a$  an element of  $\Gamma$  and, using the fact that it is linear space,  $Y^a$  also represents a vector in the tangent space  $T\Gamma$ . Given a 1-form  $\lambda_a$ , we can define a linear function of  $\Gamma$  as follows:  $F_\lambda(Y) := -\lambda_a Y^a$ . Note that  $\lambda$  is a label of the function with  $Y^a$  as its argument. First, note that there is a vector associated with  $\lambda_a$ :

$$\lambda^a := \Omega^{ab}\lambda_b$$

so we can write

$$F_\lambda(Y) = \Omega_{ab}\lambda^a Y^b = \Omega(\lambda, Y). \quad (2)$$

If we are now given another label  $\nu$ , such that  $G_\nu(Y) = \nu_a Y^a$ , we can compute the Poisson bracket

$$\{F_\lambda, G_\nu\} = \Omega^{ab}\nabla_a F_\lambda(Y)\nabla_b G_\nu(Y) = \Omega^{ab}\lambda_a \nu_b. \quad (3)$$

Since the 2-form is non-degenerate we can re-write it as  $\{F_\lambda, G_\nu\} = -\Omega_{ab}\lambda^a \nu^b$ . Thus,

$$\{\Omega(\lambda, Y), \Omega(\nu, Y)\} = -\Omega(\lambda, \nu). \quad (4)$$

As a concrete case, let us look at the example of a mechanical system whose configuration space is  $\mathcal{C} = \mathbf{R}^3$ . We can take a global chart on  $\Gamma$  given by  $(q^i, p_i)$  and consider  $\mathcal{S} = \text{Span}\{1, q^1, q^2, q^3, p_1, p_2, p_3\}$ . It is a seven-dimensional vector space. Note that we have included the constant functions on  $\Gamma$ , generated by the unit function since we know that  $\{q^i, p_j\} = \delta_j^i$ , and we want  $\mathcal{S}$  to be closed under PB.

The quantum representation is the ordinary Schrödinger picture where the Hilbert space is  $\mathcal{H} = L^2(\mathbf{R}^3, d^3x)$  and the operators are represented by

$$(\hat{1} \cdot \Psi)(q) = \Psi(q) \quad (\hat{q}^i \cdot \Psi)(q) = q^i \Psi(q) \quad (\hat{p}_i \cdot \Psi)(q) = -i\hbar \frac{\partial}{\partial q^i} \Psi(q). \quad (5)$$

Thus, we recover the conventional Schrödinger representation of the CCR.

## 2.2. Real scalar field

In this part we recall the classical theory of a real, linear Klein–Gordon field  $\phi$  with mass  $m$  propagating on a four-dimensional, globally hyperbolic spacetime  $({}^4M, g_{ab})$ . Global hyperbolicity implies that  ${}^4M$  has topology  $\mathbf{R} \times \Sigma$ , and can be foliated by a one-parameter family of smooth Cauchy surfaces diffeomorphic to  $\Sigma$  with arbitrary embeddings of the surface  $\Sigma$  into  ${}^4M$ .

The phase space of the theory can be alternatively described by the space  $\Gamma$  of Cauchy data (in the canonical approach), that is,  $\{(\varphi, \pi) | \varphi : \Sigma \rightarrow \mathbf{R}, \pi : \Sigma \rightarrow \mathbf{R}; \varphi, \pi \in C_0^\infty(\Sigma)\}$ ,<sup>1</sup> or by the space  $\mathcal{S}$  of smooth solutions to the Klein–Gordon equation which arises from initial data on  $\Gamma$  (in the covariant formalism) [6]. Note that for each embedding  $T_t : \Sigma \rightarrow {}^4M$ , there exists an isomorphism  $\mathcal{I}_t$  between  $\Gamma$  and  $\mathcal{S}$ . The key observation is that there is a one-to-one correspondence between a pair of initial data of compact support on  $\Sigma$ , and solutions to the Klein–Gordon equation on  ${}^4M$ . That is to say:

Given an embedding  $T_{t_0}$  of  $\Sigma$  as a Cauchy surface  $T_{t_0}(\Sigma)$  in  ${}^4M$ , the (natural) isomorphism  $\mathcal{I}_{t_0} : \Gamma \rightarrow \mathcal{S}$  is obtained by taking a point in  $\Gamma$  and evolving from the Cauchy surface  $T_{t_0}(\Sigma)$  to get a solution of  $(g^{ab}\nabla_a\nabla_b - m^2)\phi = 0$ . That is, the specification of a point in  $\Gamma$  is the appropriate initial data for determining a solution to the equation of motion. The inverse map,  $\mathcal{I}_{t_0}^{-1} : \mathcal{S} \rightarrow \Gamma$ , takes a point  $\phi \in \mathcal{S}$  and finds the Cauchy data induced on  $\Sigma$  by virtue of the embedding  $T_{t_0} : \varphi = T_{t_0}^*\phi$  and  $\pi = T_{t_0}^*(\sqrt{h}\mathfrak{L}_n\phi)$ , where  $\mathfrak{L}_n$  is the Lie derivative along the normal to the Cauchy surface  $T_{t_0}(\Sigma)$  and  $h$  is the determinant of the induced metric on such a surface. Note that the phase space  $\Gamma$  is of the form  $T^*\mathcal{C}$ , where the classical configuration space  $\mathcal{C}$  is comprised by the set of smooth real functions of compact support on  $\Sigma$ .

Since the phase space  $\Gamma$  is a linear space, there is a particularly simple choice for the set of fundamental observables, namely the vector space generated by *linear* functions on  $\Gamma$ . More precisely, classical observables for the space  $\Gamma$  can be constructed directly by giving smearing functions on  $\Sigma$ . We can define linear functions on  $\Gamma$  as follows: given a vector  $Y^a$  in  $\Gamma$  of the form  $Y^a = (\varphi, \pi)^a$  (note that due to the linear nature of  $\Gamma$ ,  $Y^a$  also represents a vector in  $T\Gamma$ ) and a pair  $\lambda_a = (-f, -g)_a$ , where  $f$  is a scalar density and  $g$  a scalar, we define the action of  $\lambda$  on  $Y$  as

$$F_\lambda(Y) = -\lambda_a Y^a := \int_\Sigma (f\varphi + g\pi) d^3x. \quad (6)$$

<sup>1</sup> The class of functions comprised by Schwartz space is most commonly chosen for quantum field theory in Minkowski spacetime. However, the notion of Schwartz space cannot be extended in any obvious way to more general manifolds [6, 10]. Hence, we shall define  $\Gamma$  to consist of initial data which are smooth and of compact support on  $\Sigma$ .

Now, since in the phase space  $\Gamma$  the symplectic structure  $\Omega$  takes the following form, when acting on vectors  $(\varphi_1, \pi_1)$  and  $(\varphi_2, \pi_2)$ ,

$$\Omega([\varphi_1, \pi_1], [\varphi_2, \pi_2]) = \int_{\Sigma} (\pi_1 \varphi_2 - \pi_2 \varphi_1) d^3x, \quad (7)$$

we can write the linear function (6) in the form  $F_{\lambda}(Y) = \Omega_{ab} \lambda^a Y^b = \Omega(\lambda, Y)$ , if we identify  $\lambda^b = \Omega^{ba} \lambda_a = (-g, f)^b$ . That is, the smearing functions  $f$  and  $g$  that appear in the definition of the observables  $F$  and are therefore naturally viewed as a 1-form on phase space, can also be seen as the vector  $(-g, f)^b$ . Note that the role of the smearing functions is interchanged in passing from a 1-form to a vector. Of particular importance for what follows is to consider *configuration* and *momentum* observables. They are particular cases of the observables  $F$  depending on specific choices for the label  $\lambda$ . Let us consider the ‘label vector’  $\lambda^a = (0, f)^a$ , which would normally be regarded as a vector in the ‘momentum’ direction. However, when we consider the linear observable that this vector generates, we get

$$\varphi[f] := \int_{\Sigma} d^3x f \varphi. \quad (8)$$

Similarly, given the vector  $(-g, 0)^a$  we can construct

$$\pi[g] := \int_{\Sigma} d^3x g \pi. \quad (9)$$

Note that any pair of test fields  $(-g, f)^a \in \Gamma$  defines a linear observable, but they are ‘mixed’. More precisely, a scalar  $g$  in  $\Sigma$ , that is, a pair  $(-g, 0) \in \Gamma$ , gives rise to a *momentum* observable  $\pi[g]$  and, conversely, a pair  $(0, f)^a$  yields a *configuration* observable.

### 3. Quantum scalar field

This section has two parts. In the first, we follow the algebraic quantization procedure described in the last section for the case of a Gaussian (Fock) measure. In the second part we recall the approach of [9], in which a different representation of the CCR is obtained.

*Algebraic quantization.* The algebraic quantization procedure for the scalar field, in analogy with the finite-dimensional system, starts by considering the set  $\mathcal{S}$  to be the span of the identity and the functions  $F_{\lambda}(Y)$ . The vector spaces  $V$  where the abstract operators are to be represented will be taken to be functionals of the configuration variable  $\varphi$ , that is, elements of the form  $\Psi[\varphi]$ . In analogy with quantum mechanics, the most natural representation of the basic operators, when acting on functionals  $\Psi[\varphi]$ , is as follows

$$(\hat{\varphi}[f] \cdot \Psi)[\varphi] := \varphi[f] \Psi[\varphi], \quad (10)$$

and

$$(\hat{\pi}[g] \cdot \Psi)[\varphi] := -i\hbar \int_{\Sigma} d^3x g(x) \frac{\delta \Psi}{\delta \varphi(x)} + \text{multiplicative term}. \quad (11)$$

The second term in (11), depending only on the configuration variable, is precisely there to render the operator self-adjoint when the measure is different from the ‘homogeneous’ measure, and it usually depends on the details of the measure. That is, given the quantum measure, that for free field theories is known to be ‘Gaussian’, one should adjust the action of the momentum operator in order to satisfy the reality conditions. In what follows we shall proceed with the choices that are motivated by geometrical considerations. We know that if the momentum observable can be associated with a vector field  $v^a$  on configuration space, then the general form of the momentum operator is given by  $\hat{P}(v) = -i\hbar(\mathcal{L}_v + \frac{1}{2}\text{Div}_{\mu} v)$ , where  $\text{Div}_{\mu} v$  is the divergence of the vector field  $v$  with respect to the (quantum) measure  $\mu$  (recall

that a volume element is sufficient to define the divergence of a vector field). Therefore, given the quantum measure in the field theory case, one can in principle determine the multiplicative term in the representation of the quantum momentum operator.

Let us now recall the general form of the quantum measure in the Schrödinger representation [9]. Let  $G$  be a positive Hermitian operator in the  $L^2$  Hilbert space of scalar functions  $\varphi$ . Then the general Gaussian measure is heuristically of the form

$$d\mu_G = \exp\left[-\int_{\Sigma} d^3x \varphi G \varphi\right] \mathcal{D}\varphi, \quad (12)$$

where  $\mathcal{D}\varphi$  is the fictitious homogeneous functional measure. Now, the vector fields on configuration space  $\mathcal{C}$ , associated with the momentum variables  $\pi[g]$  are constant vector fields (in the chart defined by  $(\varphi, \pi)$ ). There is a general formula for the divergence of a ‘constant’ vector field  $v^a$  given by  $\text{Div}_{\mu} v = v^a \nabla_a (\ln \mu)$ . In the infinite-dimensional case, this has to be properly reinterpreted in terms of ‘functional derivatives’. In our case, the logarithmic derivative of the measure along the constant vector field defined by  $g$  yields a quantum momentum operator of the form

$$\hat{\pi}[g] \cdot \Psi[\varphi] = -i \int_{\Sigma} \left( g \frac{\delta}{\delta \varphi} - \varphi G g \right) \Psi[\varphi]. \quad (13)$$

This completes the kinematical quantization from the algebraic point of view, for a general Gaussian measure  $\mu_G$  [10]. Note that ‘correction term’ in (13) is the most natural choice (from the infinite possibilities that the algebraic approach allows) for the momentum operator.

*GNS construction.* Let us now briefly review the results of [9]. The Fock representation of a scalar field on an arbitrary spacetime is based on the construction of a one-particle Hilbert space  $\mathcal{H}_{1-p}$ , constructed by defining a Hermitian inner product on the phase space  $\Gamma$ . In turn, this inner product can be constructed using a complex structure  $J$  on  $\Gamma$ , together with the naturally defined Symplectic structure on  $\Gamma$ :  $\mu_{\Gamma}(\cdot, \cdot) = -\Omega(\cdot, J\cdot)$ .<sup>2</sup> When the inner product  $\mu_{\Gamma}$  satisfies certain conditions, then the resulting Hilbert space can be used to construct the Fock space [6]. In the canonical picture, the complex structure has the form  $-J_{\Gamma}(\varphi, \pi) = (A\varphi + B\pi, C\pi + D\varphi)$ , where  $A, B, C, D$  are suitably defined operators on the space of initial conditions, satisfying conditions between them [12]. The inner product on  $\Gamma$  is then

$$\mu_{\Gamma}((\varphi_1, \pi_1), (\varphi_2, \pi_2)) = \int_{\Sigma} d^3x (\pi_1 B \pi_2 + \pi_1 A \varphi_2 - \varphi_1 D \varphi_2 - \varphi_1 C \pi_2).$$

The idea of the GNS construction is to start with the Weyl algebra generated by the elements of the form  $\hat{W}[\lambda] = \exp(i\hat{F}[\lambda])$  and define an *algebraic state*  $\omega$  that maps the Weyl algebra to the complex number. The GNS theorem assures us that there is a unique (up to unitary equivalence) representation of the CCR on a Hilbert space, such that the action of the state  $\omega$  on the generators of the Weyl generators can be understood as the vacuum expectation values of the Weyl operators.

The key step in the construction of the Schrödinger–Fock representation is to use the algebraic state that depends on the phase space inner product  $\mu_{\Gamma}$ . The algebraic state on an arbitrary curved spacetime then takes the form [9]

$$\omega_{\text{fock}}(\hat{W}(\lambda)) = e^{-\frac{1}{4}\mu_{\Gamma}(\lambda, \lambda)}. \quad (14)$$

<sup>2</sup> Note that we are using  $\mu$  for two different constructs:  $\mu_{\Gamma}$  represents an inner product on the phase space, and  $\mu_G$  represents a Gaussian measure on the quantum configuration space.

Then, by imposing this condition on the basic generators  $\hat{W}(\lambda)$  (corresponding to the exponentiated versions of the configuration  $\varphi[f]$  observables), one finds that the quantum measure is of the form

$$d\mu = e^{-\int_{\Sigma} \varphi B^{-1} \varphi} \mathcal{D}\varphi. \quad (15)$$

Note that the measure only knows about one of the operators defining  $J_{\Gamma}$ , namely  $B$ . One expects, however, that the full quantum theory knows about at least one other of the operators in  $J$  (two of which are independent). This expectation is realized in the representation of the momentum operator.

The strategy is to assume a general form for the momentum operator (11); one then applies condition (14) to the momentum operator  $\hat{\pi}[g]$  and makes use of the Baker–Campbell–Hausdorff relation. Then it is straightforward to show that the momentum operator takes the form

$$\hat{\pi}[g] \cdot \Psi[\varphi] = -i \int_{\Sigma} \left( g \frac{\delta}{\delta \varphi} - \varphi (B^{-1} + iB^{-1}A)g \right) \Psi[\varphi], \quad (16)$$

where  $B^{-1}$  and  $B^{-1}A$  are also Hermitian operators, and  $B^{-1}$  is the operator corresponding to  $G$  in (13). Note that the momentum operators  $\hat{\pi}[g]$  and  $\hat{\pi}[h]$  commute for any choice of  $g, h$  given that  $B^{-1}A$  is self-adjoint [9]. The most notable fact about the momentum operator thus found (16) is that it has an *extra term*, as compared to (13).

A possible worry about this term is that the operator might not satisfy the required reality conditions. However, the extra term,  $[\int_{\Sigma} \varphi (B^{-1}A)g] \Psi[\varphi]$ , being a configuration operator smeared with a real test function  $B^{-1}Ag$ , is already a Hermitian operator. Thus the reality conditions are satisfied in both representations (13) and (16). Note also that from the geometric point of view, the representation found with the algebraic perspective (13) is the most natural one, when one has a cotangent bundle structure for the phase space and one is working in the configuration representation (vertical polarization). It is indeed intriguing that one has an alternative and not so intuitive representation. What then is the relation between them? In order to explore this question let us make in the next section a brief detour into ordinary quantum mechanics where this can be easily understood. We shall come back to this question at the end of section 4.

#### 4. Unitary transformations

Let us take a mechanical system whose phase space  $\Gamma$  is given by pairs  $(q^i, p_j)$ . The canonical Poisson brackets  $\{q^i, p_j\} = \delta_j^i$  induce, via the Dirac prescription, the CCR  $[\hat{q}^i, \hat{p}_j] = i\hbar \delta_j^i$ . Now, let us suppose we have two different representations of the CCR on the *same* Hilbert space  $\mathcal{H} = L^2(q, dq)$ , given by

$$(\hat{q}^i \cdot \psi)(q) := q^i \psi(q) \quad (\hat{p}_j \cdot \psi)(q) := -i\hbar \frac{\partial}{\partial q^j} \psi(q) \quad (17)$$

and

$$(\hat{\tilde{q}}^i \cdot \psi)(q) := q^i \psi(q) \quad (\hat{\tilde{p}}_j \cdot \psi)(q) := \left( -i\hbar \frac{\partial}{\partial q^j} + q^j \right) \psi(q). \quad (18)$$

The question we want to ask is the following: is there a way of relating both representations via a *unitary transformation*? As we shall see in the following, the answer is in the affirmative. Let us recall that given a real function  $T$  on the classical phase space, the one-parameter family of diffeomorphisms generated by its Hamiltonian vector field  $X_T^a$  induces a map  $U(t)$  on the

algebra of functions on the phase space  $f \rightarrow U(t) \cdot f$  given by [13, 14]

$$\begin{aligned} U(t) \cdot f &= \sum_{n=0}^{\infty} \frac{t^n}{n!} \{f, T\}_n \\ &:= f + t\{f, T\} + \frac{t^2}{2!} \{\{f, T\}, T\} + \dots \end{aligned} \quad (19)$$

One should note that for each value of  $t$  the Poisson structure of the phase space is preserved, inducing an automorphism on the algebra of observables. The corresponding quantum operator  $\hat{U}$  should then be an automorphism in the algebra of quantum operators and therefore a unitary operator. It is clear also that it should be of the form  $\hat{U} = \exp\left[\frac{i}{\hbar}\hat{T}\right]$ , where  $\hat{T}$  is Hermitian. Given a state  $|\psi\rangle$ , by means of the operator it gets mapped to  $\hat{U}|\psi\rangle$  and any observable  $\hat{O}$  will go to  $\hat{U} \cdot \hat{O} \cdot \hat{U}^{-1}$ . In the example outlined above, it is clear that the generating function  $T$  is given by

$$T = \frac{1}{2} \left( \sum_i q^i q^i \right).$$

Therefore the automorphisms generated on the functions  $F(q, p) = \alpha_i q^i + \beta^j p_j$  are

$$F(q, p) \rightarrow F(q, p) + \beta^j q_j \quad (20)$$

thus, the elementary observables get mapped as

$$\tilde{q}^i = q^i \quad \tilde{p}_j = p_j + q_j. \quad (21)$$

The corresponding quantum unitary operator  $\hat{U}$  is given by

$$\hat{U} = \exp \left[ \frac{i}{2\hbar} \sum_i \hat{q}^i \hat{q}^i \right], \quad (22)$$

and maps the corresponding operators as follows:

$$\hat{\tilde{q}}^i = \hat{q}^i \quad \hat{\tilde{p}}_j = \hat{p}_j + \hat{q}_j. \quad (23)$$

This completes our detour into quantum mechanics.

Let us now return to our field theory problem. We have two representations given by (13) and (16) and note that they have precisely the structure of (22) and (23), where the momentum operators differ by a pure configuration observable. Therefore, the general theory of classical and quantum canonical transformations as discussed above should also apply to this system. It is straightforward to find the generating function  $T$  in the field theory case:

$$T[(\varphi, \pi)] = \frac{1}{2} \int_{\Sigma} d^3x \varphi K \varphi, \quad (24)$$

where  $K = B^{-1}A$ . Therefore it is immediate to write the corresponding would-be generator of unitary transformations,

$$\hat{U} = \exp \left[ \frac{i}{2\hbar} \int_{\Sigma} d^3x (\widehat{\varphi K \varphi}) \right]. \quad (25)$$

Then, one might be led to conclude that the representations (13) and (16) are unitarily equivalent, and therefore the algebraic procedure provides us with a correct and equivalent quantum theory to the representation found in [9].

Interestingly, this is indeed *not* the case. That is, the two representations are, in general, unitarily inequivalent. Let us now try to see why this is the case. As we have briefly explained, the quantization of the scalar field used in [9] that yields the representation (16) is based on

the GNS construction of a representation of the canonical Weyl algebra, equivalent to a given Fock representation. The representation (16) was obtained by requiring that the Weyl operators  $\hat{W}[\lambda] = \exp(i\hat{F}[\lambda])$  be unitary and whose vacuum expectation values coincide with those of the Fock representation (that knows about both operators  $G$  and  $K$ ). Then, the general representation should contain both terms in (16). Let us now consider the vacuum expectation values of the resulting quantum theories. For the GNS construction, formula (14) yields

$$\langle \hat{W}(\lambda) \rangle_{\text{gns}} = \exp \left[ -\frac{1}{4} \int_{\Sigma} d^3x (fBf + fAg - gDg - gCf) \right] \quad (26)$$

for a ‘label vector’  $\lambda^a = (g, f)^a$ . On the other hand, the representation (13) will have, as vacuum expectation values,

$$\langle \hat{W}(\lambda) \rangle_{\text{alg}} = \exp \left[ -\frac{1}{4} \int_{\Sigma} d^3x (fBf - gB^{-1}g) \right]. \quad (27)$$

From the previous expressions, it is clear that the absence of the extra term in the representation (13) implies that, in general, the vacuum expectation values (26) and (27) differ. Thus, the theories are unitarily inequivalent. This is the main observation of this letter.

It is important to stress that the main point that we want to emphasize here is the fact that theories that heuristically should be equivalent, turn out not to be. That is, one might think that under appropriate regularization procedures (given that one has product of operators), one might be able to find a unitary operator for  $\hat{U}$  in (25) on the Hilbert space of the theory. The general results of [9] tell us, however, that for certain operators  $K$ , no such regularization exists. The precise conditions under which both representations are unitarily equivalent will be reported elsewhere.

## 5. Discussion and outlook

In this letter we have analysed the canonical quantization of a real scalar field. We have shown that the quantization found by a direct application of the algebraic approach [3], using the most simple and natural choice for the representation of the CCR, is incomplete. That is, a crucial term in the representation, which is completely unnatural from the geometric-algebraic viewpoint, is missing. Furthermore, this term seems to be, at least at a heuristic level, unitarily implementable. However, more rigorous results from GNS tell us that such a unitary transformation does not exist in general. In a sense, these results illustrate a class of ambiguities in the quantization of field theories that were not explicitly considered before.

The algebraic approach to quantization is general enough that it allows for ‘any’ representation of the CCR in the Schrödinger picture. In this respect, the Fock–Schrödinger representation of [9] lies within this general scheme. However, what we have shown is that there are, in fact, an infinite number of inequivalent representations, labelled by  $K$ , that share the same Hilbert space structure (i.e. measure  $\mu_G$ ). We have also shown that the often used strategy of fixing the representation by means of the measure misses this infinite freedom. Thus, one needs some other principle to arrive at the correct representation for the system under consideration.

Let us end with three remarks.

1. This ‘negative’ result, together with recent results concerning the unitary implementability of (arbitrary) time evolution [15, 16], points in the direction that finite ‘exponentiated’ versions of (possibly) well-defined Hermitian operators might not in general exist as operators in a rigorously defined quantum field theory. Needless to say, a deeper understanding of these features is needed.

2. In the literature it is sometimes assumed that the correct representation for the momentum operator comes from equation (13). This assumption is not completely unjustified, since for the cases that are normally considered in the literature—such as Minkowski and static spacetimes, for instance—the operator  $K$  vanishes and therefore both representations coincide. It is only when one considers the most general case on curved spacetimes that such a term manifests itself.
3. In the non-perturbative quantization of general relativity [17], where one needs to define a background free quantum field theory, it is very important to have full control over the whole realm of possible ambiguities in the quantization process. The ambiguity pointed out in this letter might be of some relevance for the choice of right representation of the ‘electric field’ momentum operators in the quantum geometry formalism [18], and for analysing issues related to the semi-classical, low-energy limit of the theory.

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