Third quantization

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Abstract. The basic ideas of second quantization and Fock space are extended to density operator states, used in treatments of open many-body systems. This can be done for fermions and bosons. While the former only requires the use of a non-orthogonal basis, the latter requires the introduction of a dual set of spaces. In both cases an operator algebra closely resembling the canonical one is developed and used to define the dual sets of bases. We here concentrated on the bosonic case where the unboundedness of the operators requires the definitions of dual spaces to support the pair of bases. Some applications, mainly to non-equilibrium steady states, will be mentioned.

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1. INTRODUCTION

Second quantization has been one of the early fields of Marcos Moshinsky and his book on its applications to fermionic systems [1] has formed many of us. One of us had the pleasure to look with Marcos into the extensions of this formalism to non-orthogonal bases and the introduction of a dual basis and corresponding dual sets of operators in this context [2]. Since these concepts have become very useful for open many-body systems and recently one of us has generalized them to what may be called "third quantization" by applying second quantization and the Fock space concept to density operator spaces of mixed states and spaces of observables of fermionic systems [3]. The use of a set of dual bases becomes essential to maintain a simple algebraic form for the problem. Third quantization was successfully used to explicitly and elegantly solve situations with quadratic (or quasi-free) Hamiltonians and linear coupling to an environment via the Lindblad operators [3, 4] or via the Redfield model [5]. The next step is to follow Marcos Moshinsky to the harmonic oscillator [6], i.e. to bosonic systems [7]. This step implies not only the introduction of a dual basis, but actually of a dual space. We shall give a view of these recent developments emphasizing the elegance and efficiency of the methods more than any specific application. We shall present basis sets for the dual bases in a rather formal way and then show that it is the algebraic structure that determines the actual implementation. The implication, which this has in terms of enveloping algebras, their underlying Lie algebras and the corresponding groups has not been explored at all. Furthermore the possibilities to use graded algebras and combining fermionic and bosonic degrees of freedom in such a treatment, is very enticing to any disciple of Marcos Moshinsky. We shall here try to lay the foundations and give a taste of things to come, in the hope of enticing other participants of this meeting to help explore this line of thinking. Proceeding in reverse order of temporal development, we shall first

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present the bosonic case, with its richer structure and then go to the fermionic problem. Finally an outlook will be given on what should be done to obtain a more complete theoretical descriptions of each of the cases and for their algebraic unification.

2. BOSONIC SYSTEMS

Let us consider a Hilbert-Fock space $\mathscr{H}$ of *n bosons*. Elements of $\mathscr{H}$ can be generated from a particular element $\psi_0 \in \mathscr{H}$, called *a vacuum pure state*, and a set of *n* unbounded operators over $\mathscr{H}$, $a_1, \ldots, a_n$, which annihilate ψ_0, $a_j|\psi_0\!>= 0$, and their Hermitian adjoints $a_1^\dagger, \ldots, a_n^\dagger$, satisfying *canonical commutation relations* (CCR)

$$[a_j, a_k^\dagger] = \delta_{j,k}, \quad [a_j, a_k] = [a_j^\dagger, a_k^\dagger] = 0. \tag{1}$$

Let us define a pair of vector spaces $\mathscr{K}$ and $\mathscr{K}'$, such that $\mathscr{K}$ contains trace class operators, such as density matrices, and $\mathscr{K}'$ contains unbounded operators representing physical observables. We choose a specific space of observables $\mathscr{K}'$ and define a subspace $\mathscr{K}$ of *trace class* operators over $\mathscr{H}$, such that $\rho \in \mathscr{K}$ if and only if $A\rho$ is trace class for any $A \in \mathscr{K}'$. Thus $\mathscr{K}'$ and $\mathscr{K}$ form a dual pair of Hilbert spaces and we will later choose a dual pair of bases, one from each of these spaces.

For instance, we may chose $\mathscr{K}'$ as a linear space of all (*unbounded*) operators whose phase space representation of the operator is an entire function on the corresponding $2n-$dimensional phase space. Then $\mathscr{K}$ must be restricted to operators with finite support in the number operator basis, i.e. to operators which have a finite number of non-vanishing matrix elements in this basis. Such a constraint on density matrices may be too restrictive for certain applications. We shall show later [using eq. (9)] how this restriction can be relaxed by appropriately restricting $\mathscr{K}'$.

We now proceed with an algebraic development and conveniently adopt Dirac notation. We write an element of $\mathscr{K}$ as *ket* $|\rho\rangle$ and an element of $\mathscr{K}'$ as *bra* $(A|$, and define their contraction or scalar product to give the expectation value of A for a state ρ,

$$(A|\rho\rangle = \mathrm{tr} A\rho. \tag{2}$$

We use distinct types of brackets to emphasize the difference between the spaces from which the ket and the bra have to be chosen.

If b is any of the operators $a_j, a_j^\dagger$, then for each $\rho \in \mathscr{K}$ and $A \in \mathscr{K}'$, $b\rho, \rho b$ and Ab, bA are also elements of $\mathscr{K}$ and $\mathscr{K}'$ respectively. Thus we define the left multiplication maps $\hat{b}^{\mathrm{L}}$ and the right multiplication maps $\hat{b}^{\mathrm{R}}$ over $\mathscr{K}$ by

$$\hat{b}^{\mathrm{L}}|\rho\rangle = |b\rho\rangle, \quad \hat{b}^{\mathrm{R}}|\rho\rangle = |\rho b\rangle. \tag{3}$$

The action of their adjoint on $\mathscr{K}'$ is defined by (2) and the fact that the trace is cyclic. Thus

$$(A|\hat{b}^{\mathrm{L}} = (Ab|, \quad (A|\hat{b}^{\mathrm{R}} = (bA|. \tag{4}$$

Loosely speaking, we can also say that $(\hat{b}^{\mathrm{L}})^* = \hat{b}^{\mathrm{R}}$ and $(\hat{b}^{\mathrm{R}})^* = \hat{b}^{\mathrm{L}}$.

Next we define the set of $4n$ maps $\hat{a}_{\nu,j}, \hat{a}'_{\nu,j}, j = 1,\ldots,n, \nu = 0,1$,

$$\begin{aligned} \hat{a}_{0,j} &= \hat{a}^{\mathrm{L}}_j, \qquad \hat{a}'_{0,j} = \hat{a^{\dagger}}^{\mathrm{L}}_j - \hat{a^{\dagger}}^{\mathrm{R}}_j, \\ \hat{a}_{1,j} &= \hat{a^{\dagger}}^{\mathrm{R}}_j, \qquad \hat{a}'_{1,j} = \hat{a}^{\mathrm{R}}_j - \hat{a}^{\mathrm{L}}_j. \end{aligned} \tag{5}$$

that have the unique properties: (i) almost-canonical commutation relations

$$[\hat{a}_{\nu,j}, \hat{a}'_{\mu,k}] = \delta_{\nu,\mu}\delta_{j,k}, \quad [\hat{a}_{\nu,j}, \hat{a}_{\mu,k}] = [\hat{a}'_{\nu,j}, \hat{a}'_{\mu,k}] = 0, \tag{6}$$

(ii) $\hat{a}'_{\nu,j}$ left-annihilate the identity operator

$$(1|\hat{a}'_{\nu,j} = 0 \tag{7}$$

and (iii) $\hat{a}_{\nu,j}$ right-annihilate the vacuum pure state $|\rho_0\rangle \equiv |\psi_0><\psi_0|$

$$\hat{a}_{\nu,j}|\rho_0\rangle = 0. \tag{8}$$

Writing a $2n$ component multi-index $\underline{m} = (m_{\nu,j} \in \mathbb{Z}_+; \nu \in \{0,1\}, j \in \{1\ldots n\})^T$ we define a dual pair of Fock bases, one for each of the spaces $\mathscr{K}, \mathscr{K}'$ as

$$|\underline{m}\rangle = \prod_{\nu,j} \frac{(\hat{a}'_{\nu,j})^{m_{\nu,j}}}{\sqrt{m_{\nu,j}!}} |\rho_0\rangle, \quad (\underline{m}| = (1| \prod_{\nu,j} \frac{(\hat{a}_{\nu,j})^{m_{\nu,j}}}{\sqrt{m_{\nu,j}!}} \tag{9}$$

Their bi-orthonormality $(\underline{m}'|\underline{m}\rangle = \delta_{\underline{m}',\underline{m}}$ is directly guaranteed by the almost-CCR (6). Here and for the rest of the paper, $\underline{x} = (x_1, x_2, \ldots)^T$ designates a vector (column) of any, scalar-, operator- or map-valued symbols.

The explicit construction of the bases (9) allows us to enlarge and restrict the spaces $\mathscr{K}$ and $\mathscr{K}'$ such as to keep duality by always restricting one when extending the other or vice versa appropriately. We achieve this identifying the space $\mathscr{K}$ with the l^2 Hilbert space of vectors of coefficients $\{\sigma_{\underline{m}}\}$, $\mathscr{K} \ni |\sigma\rangle = \sum_{\underline{m}} \sigma_{\underline{m}} |\underline{m}\rangle$, and the space $\mathscr{K}'$ with the l^2 Hilbert space of vectors of coefficients $\{S_{\underline{m}}\}$, $\mathscr{K}' \ni (S| = \sum_{\underline{m}} S_{\underline{m}} (\underline{m}|$. Then, clearly by Cauchy-Schwartz inequality, $|\operatorname{tr} S\sigma| = |\sum_{\underline{m}} S_{\underline{m}} \sigma_{\underline{m}}| < \infty$ and hence $\mathscr{K}$ and $\mathscr{K}'$ are dual in the required sense.

The main idea of application of the third quantization is then to express the generators of quantum master equations, governing the dynamics of a density matrix, in terms of canonical operator maps $\hat{a}_{\nu,j}, \hat{a}'_{\nu,j}$. For quadratic systems, for example, such generators are again quadratic and can be decomposed to normal (master) modes, and thus diagonalized, by means of a non-unitary analogue of the Bogoliubov-de Gennes transformation (see [3, 5, 7]). In particular, the physically interesting *non-equilibrium-steady-state* can be constructed as the *right-vacuum* state of our theory.

3. FERMIONIC OPERATORS

In [3] the entire idea of third quantization was first presented, but the maps on the operator spaces were not given in terms of raising and lowering operators but in terms of Hermitian "coordinates" and "momenta". We shall here briefly indicate, that it can be done equally for fermionic (anti-commuting) raising and lowering operators. Thus the situation is maintained as symmetric as possible to the boson case. The main difference will naturally be, that the two bi-orthogonal bases will span the same Hilbert space rather than a dual pair.

Thus we point out an equivalent version of fermionic third quantization, which follows exactly the steps of the present communication, but starting instead from a set of fermionic operators $c_j, c_j^\dagger$, obeying *canonical anti-commutation relations* (CAR),

$$\{c_j, c_k^\dagger\} = \delta_{j,k}, \quad \{c_j, c_k\} = \{c_j^\dagger, c_k^\dagger\} = 0, \tag{10}$$

introducing the dual sets of density operators and observables, stating (2, 3,4) and defining the canonical adjoint fermionic maps

$$\begin{aligned} \hat{c}_{0,j} &= \hat{c}_j^{\mathrm{L}}, & \hat{c}'_{0,j} = \hat{c^\dagger}_j^{\mathrm{L}} - \hat{c^\dagger}_j^{\mathrm{R}} \hat{\mathscr{P}}, \\ \hat{c}_{1,j} &= \hat{c^\dagger}_j^{\mathrm{R}} \hat{\mathscr{P}}, & \hat{c}'_{1,j} = \hat{c}_j^{\mathrm{R}} \hat{\mathscr{P}} - \hat{c}_j^{\mathrm{L}}, \end{aligned} \tag{11}$$

satisfying almost-CAR

$$\{\hat{c}_{\nu,j}, \hat{c}'_{\mu,k}\} = \delta_{\nu,\mu}\delta_{j,k}, \quad \{\hat{c}_{\nu,j}, \hat{c}_{\mu,k}\} = \{\hat{c}'_{\nu,j}, \hat{c}'_{\mu,k}\} = 0, \tag{12}$$

and the properties (7,8). The parity superoperator $\hat{\mathscr{P}}$ is uniquely defined by its action on the dual vacuum states, $(1|\hat{\mathscr{P}} = (1|, \hat{\mathscr{P}}|\rho_0\rangle = |\rho_0\rangle$, and requiring that it anti commutes with all the elements of the adjoint-algebra $\{\hat{\mathscr{P}}, \underline{\hat{c}}\} = \{\hat{\mathscr{P}}, \underline{\hat{c}}'\} = 0$. The difference to the more symmetric approach [3] is that now the canonical conjugate adjoint maps are *not* the hermitian adjoint maps $\hat{c}'_{\nu,j} \neq \hat{c}^\dagger_{\nu,j}$, which is however of no consequence as we are anyway dealing with problems in which *non-normal* operators enter in an essential way. The complete bi-orthogonal bases of the density operator space $\mathscr{K}$, and its dual, the space of observables $\mathscr{K}'$, analogue to (9), can now be labelled by means of binary multi indices $\underline{m}$, $m_{\nu,j} \in \{0, 1, \}$,

$$|\underline{m}\rangle = \prod_{\nu,j} (\hat{c}'_{\nu,j})^{m_{\nu,j}} |\rho_0\rangle, \quad (\underline{m}| = (1| \prod_{\nu,j} (\hat{c}_{\nu,j})^{m_{\nu,j}} \tag{13}$$

4. CONCLUSIONS

We have presented third quantization for bosonic and fermionic operators states, attempting a uniform presentation. The result in itself is remarkable and very useful, but was essentially taken form refs [3, 5, 7]. The purpose of this presentation was to show the structure of the formalism presented in a form which prepares the use of algebraic and group theoretical techniques along the lines developed by Marcos Moshinsky. Operator states were not known and non-orthogonal bases were rarely used in this context, but in [2] Marcos Moshinsky together with one of the authors developed the latter for fermionic systems in second quantization. Even there advantage was taken of the fact, that the algebraic structure defines the important features of the problem. Thus combining raising operators in the dual basis with lowering operators in the original one, one could mimic the algebraic structure developed for standard anti commuting operators. This clearly carries over to the third quantized picture. For bosonic systems the situation is a little more involved because we deal with operators on different spaces, yet we feel confident, that we can develop the techniques known as dynamical algebras or spectrum generating algebras also in this case, though the central interest clearly is not on any spectrum. The entire idea relies on the point that through bases (9) and (13) we can pass to equivalent infinite l^2 spaces in the first case and finite ones in the second. Limiting algebraic operations appropriately we never see the differences or they appear in the occasional use of an overlap matrix or its inverse. Note that the freedom we have in the fermionic case is larger than in the bosonic one, as we are never in danger of leaving the finite dimensional Hilbert space.

Summarizing we may say that the construction we present provides an ideal framework for algebraic or group-theoretical developments. Yet filling the framework has barely begun. It also seems obvious that we can construct graded algebras also known as superalgebras, mixing anti-commuting and commuting variables, in the present context.

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