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QUANTUM COMPUTING AND SECOND QUANTIZATION

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Abstract

Quantum computers are by their nature many particle quantum systems. Both the many-particle arrangement and being quantum are necessary for the existence of the entangled states, which are responsible for the parallelism of the quantum computers. Second quantization is a very important approximate method of describing such systems. This lecture will present the general idea of the second quantization, and discuss shortly some of the most important formulations of second quantization.

Keywords: Quantum mechanics, quantum computing, second quantization, multiparticle quantum theory

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1 Motivation

Quantum computing is a relatively new paradigm for computing, with basis in quantum mechanics [1]. Second quantization is a very important technique within quantum mechanics [2] (and even more important in quantum field theory). The question I will attempt to answer is are there any applications of second quantization in quantum computing. I present a very brief account of some aspects of both second quantization and quantum computing, reflecting my own interests. I also discuss potential and actual points of contact between second quantization and quantum computing. There are interesting and not fully understood relationships between second quantization and topology, which I stress on the way, because the large part of the readers are topologists.

The direct motivation for the work can be defined by general (birds-eye) view and more detailed (frogs-eye) view.

Birds-eye view: Multi-particle quantum mechanics and quantum field theory require more involved approach than one-particle quantum mechanics; the second quantization provides a multiparticle model. Talking about second quantization one should keep in mind that this notion means many different things. I will discuss this ambiguity later.

Frogs-eye view: Natural parallelism of calculations is the most important advantage of a quantum computer over a classical one. The parallelism is possible due to the entangled states. The entangled states are general elements of the tensor product of one-particle Hilbert spaces.

2 One-particle, nonrelativistic quantum mechanics

I summarize here briefly the standard approach, like e.g. [3], to one-particle nonrelativistic quantum mechanics.

The state of a quantum one-particle system is described by a vector in a complex Hilbert space, $\mathcal{H}$, often taken as the space

$$\mathcal{H} = L^2(X) \tag{2.1}$$

where X is (a subset of) $\mathbb{R}^D$, where $D \leq 3$. The state evolves in time

$$\psi(t, \vec{x}) = e^{it\hat{H}}\psi(0, \vec{x}) \tag{2.2}$$

where: $\hat{H} : \mathcal{H} \to \mathcal{H}$ is a self-adjoint operator in $\mathcal{H}$, often taken as

$$\hat{H} = -\frac{\hbar^2}{2m}\Delta + V(\vec{x}) \tag{2.3}$$

which corresponds to the classical one-body Hamiltonian

$$H = \frac{\vec{p}^2}{2m} + V(\vec{x}) \tag{2.4}$$

where the position becomes the operator of multiplication by the position vector,

$$\hat{\vec{x}} = \vec{x}\cdot \tag{2.5}$$

and the momentum operator becomes the differential operator

$$\hat{p} = \frac{\hbar}{i}\nabla \tag{2.6}$$

which leads to commutation relations

$$[x_i, p_j] = i\hbar\delta_{ij} \tag{2.7}$$

responsible for celebrated uncertainty relations.

Remarks:

- This is the standard theory. Different levels of deviation from the standard exist.
- Using "wave functions" with values in $\mathbb{C}$ we neglect internal degrees of freedom like spin, description of which requires consideration of multicomponent Hilbert spaces.
- Nonrelativistic particles with spin are described by a two-component wave function, or a wave function with values in $\mathbb{C}^2$

3 Second quantization as a special basis in one-particle theory

There are various "second quantizations": "second quantization" as building multi-particle quantum theory from one-particle theory; "second quantization" as introducing a special basis in the one-particle theory. In this section I discuss the second of these alternatives. Let me remind the fundamental example, which is the quantum harmonic oscillator. Let

$$\mathcal{H} = L^2(\mathbb{R}) \tag{3.1}$$

, since for simplicity I consider the $1D$ case, but it is easy to generalize to higher dimensions. Let the Hamiltonian be quadratic in momentum operator and has the potential energy quadratic in position operator. Such choice is called the "harmonic oscillator".

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 \tag{3.2}$$

Introducing a complex-linear combination of operators $\hat{x}$ and $\hat{p}$,

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} + \frac{i}{\sqrt{2m\hbar\omega}}\hat{p} \tag{3.3}$$

leads to

$$\hat{a}^* = \sqrt{\frac{m\omega}{2\hbar}}\hat{x}^* - \frac{i}{\sqrt{2m\hbar\omega}}\hat{p}^* = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} - \frac{i}{\sqrt{2m\hbar\omega}}\hat{p} \tag{3.4}$$

since

$$\hat{x}^* = \hat{x} \qquad and \qquad \hat{p}^* = \hat{p} \tag{3.5}$$

Then

$$\begin{aligned} \hat{a}^*\hat{a} &= \Big(\sqrt{\frac{m\omega}{2\hbar}}\hat{x} - \frac{i}{\sqrt{2m\hbar\omega}}\hat{p}\Big)\Big(\sqrt{\frac{m\omega}{2\hbar}}\hat{x} + \frac{i}{\sqrt{2m\hbar\omega}}\hat{p}\Big) = \\ &= \frac{m\omega}{2\hbar}\hat{x}^2 + \frac{1}{2m\hbar\omega}\hat{p}^2 + \frac{i}{2\hbar}[\hat{x},\hat{p}] = \\ &= \frac{1}{\hbar\omega}\hat{H} - \frac{1}{2}\hat{1} \end{aligned} \tag{3.6}$$

The above relationship can be rewritten as follows

$$\hat{H} = \hbar\omega\Big(\hat{a}^*\hat{a} + \frac{1}{2}\hat{1}\Big) \tag{3.7}$$

In a particular basis in the Hilbert space $\mathcal{H} = L^2(X)$, numbered by integers, $|n>$, $n = 0, 1, \cdots$, chosen as follows:

$$\hat{a}|n> = \sqrt{n}\,|n-1> \tag{3.8}$$

$$\hat{a}^*|n> = \sqrt{n+1}\,|n+1> \tag{3.9}$$

the action of appropriate operators reads

$$\hat{a}^*\hat{a}|n> = n\,|n> \tag{3.10}$$

$$\hat{H}|n> = \Big(n + \frac{1}{2}\Big)\hbar\omega \tag{3.11}$$

The operators $\hat{a}$ and $\hat{a}^*$ are called the annihilation and creation operators, respectively, due to above properties. Since in many cases the potentials of interactions can be approximated by quadratic formulas, a simple generalization of the above procedure works in these cases. However, when the quadratic approximation is not sufficient and should be corrected by higher order terms, the basis can still be applied to develop a perturbative calculus.

Feynman diagrams is a technique that provides a graphical way to represent complicated analytical expressions in such cases.

Another possibility for introducing second quantization is when the Hamiltonian of the system enjoys a symmetry. Then the Hilbert space of the system is built from the spaces of representations of the group (or, in generalized case, e.g. a quantum group). Then the intertwiners of the representations play a role analogous to the creation and annihilation operators of the kind discussed above.

Remark: The latter approach allowed for studying the problem of decoherence and prevention of decoherence in quantum computers with so called dynamical symmetry, see [4], [5].

4 Second quantization as multiparticle quantum theory

The extension of one-particle quantum mechanics to systems of many particles requires revision of the above scheme. When there are a number of particles, and the number can be changing, the Hilbert space appropriate for the description of such system is the direct sum of (square-integrable) functions of time and all N positions of particles, over the (changing) number N, [6]

$$\mathcal{F} = \bigoplus_{N\geq 0} L^2(X^N) \tag{4.1}$$

where $X \subset \mathcal{R}^D$, $D \geq 3$, $X^N = X \times X \times \cdots \times X$. The Hilbert space introduced above, or its generalization

$$\mathcal{F}(\mathcal{H}) = \bigoplus_{N\geq 0} \mathcal{H}^N \tag{4.2}$$

is called the Fock space.

For any $f \in \mathcal{H}$ one can define creation and annihilation operators on $\mathcal{F}(\mathcal{H})$, $\hat{a}^*(f)$, $\hat{a}(f)$ by

$$\begin{aligned} \hat{a}(f)\psi^{(0)} &= 0, \\ \hat{a}^*(f)\psi^{(0)} &= f \end{aligned} \tag{4.3}$$

and

$$\begin{aligned} \hat{a}(f)\Big(f_1 \otimes f_2 \otimes \cdots \otimes f_N\Big) &= \sqrt{N}\big(f, f_1\big) f_2 \otimes \cdots \otimes f_N \\ \hat{a}^*(f)\Big(f_1 \otimes f_2 \otimes \cdots \otimes f_N\Big) &= \sqrt{N+1} f \otimes f_2 \otimes \cdots \otimes f_N \end{aligned} \tag{4.4}$$

Quantum particles are not distinguishable, therefore they are described by subspaces of the Fock space, which are unitary representations of the respective permutation groups. As a result there are two kinds of particles, bosons and fermions, described by functions symmetric or antisymmetric with respect to permutations of particles. The above constructions of the Fock space and of the creation and annihilation operators split as follows

$$\mathcal{F}_{\pm}(\mathcal{H}) = P_{\pm}\mathcal{F}(\mathcal{H}) \tag{4.5}$$

where $P_{\pm}$ are projections to $\mathcal{F}_{\pm}(\mathcal{H})$, given by extensions of

$$P_+\Big(f_1 \otimes f_2 \otimes \cdots \otimes f_N\Big) = \frac{1}{N!}\sum_{\pi} f_{\pi_1} \otimes f_{\pi_2} \otimes \cdots \otimes f_{\pi_N} \tag{4.6}$$

$$P_-\Big(f_1 \otimes f_2 \otimes \cdots \otimes f_N\Big) = \frac{1}{N!}\sum_{\pi} \epsilon_\pi f_{\pi_1} \otimes f_{\pi_2} \otimes \cdots \otimes f_{\pi_N} \tag{4.7}$$

where ϵ_π is the sign of the permutation of N element π.

Introduction of the subspaces of the Fock space implies introduction of creation and annihilation operators acting in the respective subspaces as follows:

$$\hat{a}_\pm(f) = P_\pm \hat{a} P_\pm \tag{4.8}$$

$$\hat{a}^*_\pm(f) = P_\pm \hat{a}^* P_\pm \tag{4.9}$$

where $f \in \mathcal{H}$.

In the case when $\mathcal{H} = L^2(X)$, there could be defined the creation and annihilation operators depending on position, as follows:

$$\left(\hat{a}_\pm(\vec{x})\,\psi\right)^{(N)}(\vec{x}_1, \vec{x}_2, \ldots, \vec{x}_N) = \sqrt{N+1}\,\psi^{(N+1)}(\vec{x}, \vec{x}_1, \vec{x}_2, \ldots, \vec{x}_N) \tag{4.10}$$

$$\left(\hat{a}^*_\pm(\vec{x})\,\psi\right)^{(N)}(\vec{x}_1, \vec{x}_2, \ldots, \vec{x}_N) = \tag{4.11}$$

$$= \frac{1}{\sqrt{N}} \sum_{i=1}^{N} (\pm 1)^{i-1} \delta(\vec{x} - \vec{x}_i)\,\psi^{(N-1)}(\vec{x}_1, \ldots, \hat{\vec{x}}^i, \ldots, \vec{x}_N)$$

It is clear that in fermionic case repeted application of the same creation operator leads to zero, since due to signs in the definition all terms in the resulting sum will meet the identical counterparts with opposite sign.

Digression

The latter formulas (for fermions) share too much with certain formulas for chain complexes that, in my opinion, it would be a mere coincidence. Namely, in an abstract simplicial complex consisting of a set of vertices V, a set of simplexes $P \subset 2^V$, n vertices defines, in general case, an $n-1$-dimensional simplex. Then a chain complex is defined as:

$$C_{n-1} = \tag{4.12}$$

$$= span\Big\{(v_1, v_2, \ldots, v_n) \in V^n | v_1 < v_2 < \ldots < v_n, \{v_1, v_2, \ldots, v_n\} \in P\Big\}$$

$$\partial_{n-1} : C_{n-1} \to C_{n-2} \tag{4.13}$$

$$\partial_{n-1}(v_1, v_2, \ldots, v_n) = \sum_{i=1}^{n} (-1)^{i-1} (v_1, \ldots, \hat{v}_i, \ldots, v_n) \tag{4.14}$$

Remark: Second quantization and quantum field theory Second quantization is of extreme importance in quantum field theory. Although quantum field theory is beyond the scope of this short review, it is difficult not to mention it. As a matter of fact, relativistic version of quantum mechanics suffers so many interpretation difficulties that it is a general consensus that quantum field theory has to be used in its place. Second quantization is sort of built-in in the relativistic quantum field theory. It is particularly successful in describing quantum theory of electrodynamic field, see e.g. [7], [8].

Quantum field theory and thus second quantization language is indispensable in modern quantum chromodynamics as well as in all unified field theories. The path integral approach turned out to be a basis for this development, which allows quite intuitive perturbative approaches in the nonlinear theories, see e.g. [9]. We should mention also the technique of Feynman diagrams developed as a graph theoretic means of doing calculations in the perturbative approach to quantum field theory

Second quantization can be also developed in nonrelativistic quantum field theory, where it is applicable in condensed matter physics contexts, [10].

5 Which second quantization is related to quantum computing?

I reminded two different notions of second quantization. Which of them, if any, is then related to quantum computing? The answer to this question is not as straightforward as one might think. There is no place here for thorough discussion, I will only make some points.

First, let me remind briefly certain facts about quantum computing. In quantum computing the position degrees of freedom as a rule do not play a role, but rather the internal degrees of freedom (e.g. spin) are employed, so that the many-particle quantum theory of computing deals with tensor products of the space $\mathcal{C}^2$. The elements of the two-dimensional space are called qubits (there are more general schemes, with higher- but finite-dimensional complex spaces, defining qutrits, and their higher-dimensional counterparts, e.g.) Quantum computing deals with entangled states of the qubits (general elements of the tensor product space).

Although above scheme looks like following the standard construction in the second quantization, it is not exactly so. Namely, qubits do not satisfy either bosonic or fermionic commutation rules. As is elegantly shown in [**?**, **?**] they are rather described by a parafermionic statistics, in which the creation and annihilation operators for different locations (or different modes) commute, while the operators "at the same location" (or of the same mode) satisfy fermionic anticommutation rules. A generalization of the qubit case exist, and leads to generalized parafermions, with which one can perform quantum computation [**?**, **?**]. The problems with connecting the parafermions (or qudits) with the standard second quantization is visible in the paper [13], where certain problems with constructing exchange gates are treated in qudit case and in standard second quantization case, and these are different problems, requiring different treatment.

There is another approach, using a connection between a fermionic Fock space and spaces of representation of the Spin groups, where Spin groups are considered as subsets of Clifford algebras. Orbits of the Spin groups classify spinors. Particular orbits are connected with the notion of pure spinors, for which the isotropic spaces of vectors killing the distinguished spinor has maximal dimension. Other orbits describe spinors with different levels of generalized purity, depending on the dimension, see e.g. [14].

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