CHINESE JOURNAL OF PHYSICS VOL. 35, NO. 6-11 DECEMBER 1997

Operator Space of a Quantum System

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(Received October 16, 1997)

All linear operators of a quantum system form a linear operator space. We define the inner product of two operators in the operator space and present the concepts of orthogonality and normalization of operators. Quantum description of a physical system in the operator space is demonstrated briefly.

PACS. 03.65.-w – Quantum mechanics.
PACS. 03.65.Bz – Foundations, theory of measurement, miscellaneous theories.
PACS. 03.65.Ca – Formalism.

I. Introduction

In quantum mechanics, physical systems are customarily described by state vectors, or equivalently wave functions, in the Hilbert space, and physical quantities are referred to by expectation values of self-adjoint operators, i.e., observables. Instead of working in the Hilbert space formed by all state vectors of a quantum system, we may formulate quantum mechanics directly in the operator space composed of all operators associated with the quantum system. However, the operator space of a quantum system may have been tacitly implied but has never been mentioned explicitly in both older and more recent text books on quantum mechanics [1-9]. After all, the most general state of a quantum system can only be described by the density operator, commonly known as the density matrix. Furthermore in the case of a pure state, a density operator just-describes the state of a quantum system, while a state vector over-describes the state by having an arbitrary phase factor.

In Section II, we introduce the operator space of a quantum system and define the inner product of two operators in the operator space. In Section III, we present the concepts of orthogonality and normalization of operators. The expansion theorem for an arbitrary operator in the operator space is also given. Quantum description of a physical system in the operator space is demonstrated briefly in Section IV. Conclusion is made in Section V.

II. The operator space of a physical system

II-l. Orthonormal basis states

Let $\{|i>; i = 1, 2, \cdots\}$ be a complete set of orthonormal basis states for the Hilbert space 1-I of a physical system. The basis states satisfy the orthonormal and completeness relations:

$$\langle i|j\rangle = \delta_{ij},$$
$$\sum |i\rangle\langle i| = I,$$

where I is the identity operator in the same space $\mathcal{H}$.

If the basis states are given by continuum states, the Kronecker-δ normalization in the orthonormal relation will be replaced by the Dirac-δ normalization, and the summation in the completeness relation replaced by an integration. Consider, for example, position basis states for a spinless particle in the real 3-dimensional space R^3:

$$\{|\boldsymbol{x}>; \boldsymbol{x} \in R^3\}.$$

The orthonormal and completeness relations are

$$\langle \boldsymbol{x}'|\boldsymbol{x}\rangle = \delta^3(\boldsymbol{x}' - \boldsymbol{x}),$$

$$\int d^3x |\boldsymbol{x}\rangle\langle \boldsymbol{x}| = I.$$

II-2. Operator in terms of outer products of basis states

It is convenient to express any operator Ω in terms of outer products $|i><j|$ of basis states as

$$\Omega = \sum_{ij} |i\rangle\langle i|\Omega|j\rangle\langle j|$$
$$= \sum_{ij} \omega_{ij} |i\rangle\langle j|,$$

where the set of expansion coefficients $\{\omega_{ij}\}$ is called the kernel of the operator Ω in the basis $\{|i\rangle; i = 1,2,\ldots\}$,

$$\omega_{ij} = \langle i|\Omega|j\rangle.$$

11-3. Trace of an operator

The trace of an operator Ω in the Hilbert space $\mathcal{H}$ is defined as

$$tr\{\Omega\} = \sum_i \langle i|\Omega|i\rangle \text{ for a discrete basis,}$$
$$= \int d^3x \langle \boldsymbol{x}|\Omega|\boldsymbol{x}\rangle \text{ for a continuum basis.}$$

Any operator Ω which can be reduced to the form $\Omega = |\phi\rangle\langle\phi|$ with $|\phi\rangle$ being a normalized state has a unit trace:

$$\mathrm{tr}\{\Omega\} = \mathrm{tr}\{|\phi\rangle\langle\phi|\} = \langle\phi|\phi\rangle = 1.$$

Any operator Λ which can be reduced to the form $A = |\phi\rangle\langle\psi|$ with $|\phi\rangle$ and $|\psi\rangle$ being orthogonal states is traceless:

$$\mathrm{tr}\{\Lambda\} = \mathrm{tr}\{|\phi\rangle\langle\psi|\} = \langle\psi|\phi\rangle = 0.$$

We note that the trace of the product AB of two arbitrary operators A and B equals the trace of the product BA:

$$\mathrm{tr}\{AB\} = \mathrm{tr}\{BA\}.$$

11-4. The operator **space**

The linear operator space formed by all linear operators in the Hilbert space of a quantum system is called the operator space $\mathcal{O}$ of the quantum system.

11-5. Inner product of two operators

The inner product, or contraction, of operators Ω and Λ in the operator space $\mathcal{O}$, denoted as $(\Omega|\Lambda)$, is defined to be

$$(\Omega|\Lambda) \equiv \mathrm{tr}\{\Omega^\dagger\Lambda\},$$

which is in general a complex number. Here we have borrowed the Dirac bra-ket notations with rounded brackets. We may consider $|\Lambda)$ as a ket operator in the operator space $\mathcal{O}$, and $(\Omega|$ as a bra operator in the dual operator space $\mathcal{O}'$. We note that

$$\begin{aligned}(\Lambda|\Omega) &\equiv \mathrm{tr}\{\Lambda^\dagger\Omega\}\\ &= (\Omega|\Lambda)^*.\end{aligned}$$

The inner product of two operators is a real number if both operators are self-adjoint, and the inner product of an operator with itself is also a real number.

In summary, the inner product of two operators Ω and A is a bilinear functional satisfying the following axioms:

(i) $(\Omega|\Omega) \geq 0$, and 0 only for $\Omega = 0$,
(ii) $(\Omega|\Lambda) = (\Lambda|\Omega)^*$,
(iii) $(\Omega|\alpha\Lambda + \beta\Sigma) = \alpha(\Omega|\Lambda) + \beta(\Omega|\Sigma)$,

which are analogous to axioms for the inner product of two vectors in the Hilbert space.

III. The expansion theorem in the operator space

III-l. Orthogonality between two operators

Two operators Ω and A in the operator space $\mathcal{O}$ of a quantum system are said to be orthogonal to each other if the inner product of the two operators vanishes, i.e., their product $\Omega^\dagger\Lambda$ is traceless in the space:

$$\begin{aligned}(\Omega|\Lambda) &\equiv \mathrm{tr}\{\Omega^\dagger\Lambda\}\\ &= \sum\langle i|\Omega^\dagger\Lambda|i\rangle = 0,\end{aligned}$$

where the trace may involves an integration over the continuum part of the spectrum.

If two operators Ω and A are orthogonal to each other, their kernels satisfy the relation

$$\mathrm{tr}\{\Omega^\dagger\Lambda\} = \sum_i \sum_j \omega_{ij}^* \lambda_{ij} = 0,$$

which implies also

$$\mathrm{tr}\{\Lambda^\dagger\Omega\} = \sum_i \sum_j \lambda_{ij}^* \omega_{ij} = \mathrm{tr}\{\Omega^\dagger\Lambda\}^* = 0.$$

It is of interest to note that an operator A is orthogonal to the identity operator I if and only if the operator A is traceless:

$$\mathrm{tr}\{I\Lambda\} = \mathrm{tr}\{\Lambda\} = 0.$$

111-2. Normalization of an operator

The norm of an operator Ω is defined as the square root of the inner product of the operator Ω with itself:

$$\|\Omega\| = \sqrt{(\Omega|\Omega)} = \sqrt{\mathrm{tr}\{\Omega^\dagger\Omega\}}.$$

We note that $\mathrm{tr}\{\Omega^\dagger\Omega\}$ is positive definite, i.e., always real and non-negative:

$$\begin{aligned}\mathrm{tr}\{\Omega^\dagger\Omega\} &= \sum_i \sum_j \omega_{ij}^* \omega_{ij} \\ &= \sum_i \sum_j |\omega_{ij}|^2 \geq 0.\end{aligned}$$

An operator Ω is said to be normalized if it has a unit norm:

$$\|\Omega\| = 1.$$

Any operator which has a finite norm can always be normalized by applying a multiplication factor. There are certain operators which do not have a finite norm but can be normalized with Dirac-6 functions.

111-3. Orthonormal operators

If operators $\{\Omega, \mathrm{A}, \Sigma, \ldots\}$ are each normalized and orthogonal among themselves, they form a set of orthonormal operators.

111-4. A complete set of orthonormal basis operators

The fundamental outer products $\{|i\rangle\langle j|; i, j = 1, 2, \cdots\}$ of a quantum system constitute a complete set of orthonormal basis operators,

$$\mathrm{tr}\{(|i\rangle\langle j|)^\dagger(|k\rangle\langle l|)\} = \delta_{ik}\delta_{jl},$$

by which an arbitrary operator of the quantum system may be expanded. The completeness of this set of orthonormal basis operators is implied by the completeness of the basis states: $\sum |i\rangle\langle i| = \mathrm{I}$.

111-5. The expansion theorem

Let $\{T_\alpha; \alpha = 1, 2, \cdots\}$ be a complete set of orthogonal basis operators in the operator space $\mathcal{O}$ of a quantum system, where the subscript a in T_α may represent an aggregate of several indices. An arbitrary operator Ω of the quantum system in the same space $\mathcal{O}$ may be expanded by these basis operators as

$$\Omega = \sum_\alpha \omega_\alpha T_\alpha,$$

where the expansion coefficients ω_α may be evaluated as

$$w_\alpha = \frac{\mathrm{tr}\{T_\alpha^\dagger \Omega\}}{\mathrm{tr}\{T_\alpha^\dagger T_\alpha\}}.$$

IV. Operator description of a quantum system

IV-l. Density operator in terms of orthogonal basis operators

The density operator p of a quantum system in a given operator space $\mathcal{O}$ may be expanded in a complete set of orthogonal basis operators $\{T_\alpha; \alpha = 1, 2, \cdots\}$ in the same space $\mathcal{O}$ as

$$\rho = \sum_\alpha \rho_\alpha T_\alpha,$$

where the kernel $\{\rho_\alpha\}$ of the density operator ρ may be evaluated by

$$Pa = \frac{}{\mathrm{tr}\{T_\alpha^\dagger T_\alpha\}} \mathrm{tr}\{T_\alpha^\dagger \rho\}.$$

If a particular basis operator T_α is self-adjoint, the corresponding expansion coefficient ρ_α is real because of the self-adjointness of the density operator ρ. If all the basis operators T_α are self-adjoint, then all self-adjoint operators, including density operators and observables, may be given as "vectors" with real components in the operator space.

IV-2. Expectation values of operators

The total probability Prob{p} of a quantum state described by the density operator ρ may be written as the inner product of the density operator ρ with the identity operator I:

$$\mathrm{Prob}\{\rho\} = \mathrm{tr}\{\rho\} = (\rho|I).$$

When describing the initial state of a quantum system in a certain physical process, the density operator ρ is usually scaled with $(\rho|I) = 1$ to make Prob{p} unity.

The expectation value of an arbitrary operator Ω for the quantum state described by the density operator ρ may be considered as the ratio of two inner products $(\rho|\Omega)$ and $(\rho|I)$:

$$\langle \Omega \rangle = \frac{\mathrm{tr}\{\rho\Omega\}}{\mathrm{tr}\{\rho\}} = \frac{(\rho|\Omega)}{(\rho|I)}.$$

In terms of the respective kernels $\{\rho_\alpha\}$ and $\{\omega_\alpha\}$ of ρ and Ω, we have

$$\langle\Omega\rangle = \frac{1}{\sum_\alpha \rho_\alpha \mathrm{tr}\{T_\alpha\}} \sum_\alpha \rho_\alpha^* \omega_\alpha \mathrm{tr}\{T_\alpha^\dagger T_\alpha\}.$$

It is of interest to note that the expectation value of an arbitrary operator Ω for a quantum state vanishes, if and only if the density operator ρ describing the quantum state is orthogonal to the operator Ω:

$$\langle\Omega\rangle = 0 \;\Leftrightarrow\; (\rho|\Omega) = 0.$$

If the density operator ρ is scaled with $(\rho|I) = 1$, and the basis operators T_α are orthonormal, the expectation value of the observable Ω for the quantum state ρ reduces to

$$\langle\Omega\rangle = (\rho|\Omega) = \sum_\alpha \rho_\alpha^* \omega_\alpha,$$

The expectation value of a self-adjoint operator, *e.g.*, observable Ω, has two alternative forms:

$$\langle\Omega\rangle = \frac{(\rho|\Omega)}{(\rho|I)} = \frac{(\Omega|\rho)}{(I|\rho)},$$

which is real.

V. Conclusion

We have introduced the operator space of a quantum system and defined the inner product of two operators. Every operator of the quantum system may be looked upon as a "vector" in the operator space. By choosing a complete set of self-adjoint orthonormal basis operators, we can express density operators and all observables of the quantum system as vectors with "real" components in the operator space. The expectation value of an observable Ω of the quantum system in the state described by the unity-scaled density operator ρ is simply the inner product $(\Omega|\rho)$ of the two "vectors" Ω and ρ, *i.e.*, the projection of the "vector" ρ along the "vector" Ω. The operator space could provide an alternative perspective to the quantum description of a physical system.

Acknowledgement

This work is supported in part by the National Science Council of the Republic of China under Grant No. NSC87-2112-M001-001.

References

[1] P. A. M. Dirac, *The Principles of Quantum Mechanics* (Clarendon, Oxford, 1958), *4th* ed..
[2] J. von Neumann, *Mathematical Foundations of Quantum Mechanics* (Princeton Univ., Princeton, New Jersey, 1955).
[3] A. Messiah, *Quantum Mechanics* (Wiley, New York, 1966), Vols. I and II.
[4] L. I. Schiff, *Quantum Mechanics* (McGraw-Hill, New York, 1968), *3rd* ed..

[5] V. B. Beretetskii, E. M. Lifshitz, and L. P. Pitaevskii, *Relativistic Quantum Theory,* Part 1, (Pergamon, Oxford, 1979); E. M. Lifshitz and L. P. Pitaevskii, *Relativistic* Quantum *Theory,* Part 2 (Pergamon, Oxford, 1973).

[6] C. Cohen-Tannoudji, B. Diu, and F. Laloë, Quantum *Mechanics* (Wiley, New York, 1977), Vols. I and II.

[7] R. Shankar, *Principles of Quantum Mechanics* (Plenum, New York, 1994), *2nd* ed..

[8] W. Greiner, Quantum Mechanics-An *Introduction* (Springer-Verlag, Heidelberg, 1994), *3rd* ed..

[9] D. J. Griffiths, *Introduction to* Quantum *Mechanics* (Prentice Hall, Englewood Cliffs, New Jersey, 1995).