Report 1.1: Quantum Operators

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Abstract

This note is a collection of exercises and solutions on quantum operators in the context of mathematical modeling. The problems were generated by chatGPT after providing the model with Baragrello's textbook as reference.

1 The Bosonic Number Operator

Problem: Consider a system of L bosonic modes described by the operators a_l and $a_l^\dagger$, satisfying the commutation relations:

$$[a_l, a_n^\dagger] = \delta_{ln}\mathbb{I}, \quad [a_l, a_n] = [a_l^\dagger, a_n^\dagger] = 0$$

Show that the number operator $\hat{N} = \sum_{l=1}^{L} a_l^\dagger a_l$ is self-adjoint and find its action on the Fock state $|n_1, n_2, \ldots, n_L\rangle$.

Proof. The total number operator $\hat{N}$ can be expressed as a sum of number operators for each states. Define

$$\hat{n}_l \ := \ a_l^\dagger a_l \tag{1.1}$$

then, this auxillary number operator for state l recovers the number of particles in state l.

We first recall how a Fock state is constructed. Given a set of operators $\{a_l, a_l^\dagger | 1 \leq l \leq L\}$, there exists a vaccum state ϕ_0 where $a_l\varphi_0 = 0$ for all $0 \leq l \leq L$. The Fock state $|n_1, \ldots, n_L\rangle$ is defined as

$$\varphi_{n_1,\ldots,n_L} \ := \ |n_1, \ldots, n_L\rangle \ := \ \frac{1}{\sqrt{n_1! \ldots n_L!}}(a_1^\dagger)^{n_1} \cdots (a_L^\dagger)^{n_L}\varphi_0 \tag{1.2}$$

The intution behind the construction is that the operators $a_l^\dagger$ corresponds to the creation operators, and the a_l to the anhilation operators. Thus, if the Fock state has n_l particles in state l, then the state can be recovered from the vaccum state by adding n_l creation operators. The reciprocal of the sqareroot of the factorials ensure that the state is normalized, i.e. $\|\varphi_{n_1,\ldots,n_L}\| = \|\varphi_0\| = 1$.

We now show that

$$\hat{n}_l|n_1, \ldots, n_L\rangle \ = \ n_l|n_1, \ldots, n_L\rangle. \tag{1.3}$$

It suffices to show that

$$(a_l^\dagger a_l)(a_l^\dagger)^{n_l}\varphi_0 \ = \ n_l(a_l^\dagger)^{n_l}\varphi_0 \tag{1.4}$$

since each operator corresponding to different states commute. We prove this by induction. For simplicity, we drop the subscripts and write a, n instead of a_l, n_l. Induct on n. For the base case,

$$(a^\dagger a)(a^\dagger)^0\varphi_0 \;=\; 0 \tag{1.5}$$

since the vaccum is anhilated by a. For the inductive step, consider the following.

$$(a^\dagger a)(a^\dagger)^n\varphi_0 \;=\; a^\dagger(aa^\dagger)(a^\dagger)^{n-1}\varphi_0 = a^\dagger(I + a^\dagger a)(a^\dagger)^{n-1}\varphi_0 \tag{1.6}$$

$$= \;(a^\dagger)^n\varphi_0 + (a^\dagger a)(a^\dagger)^{n-1}\varphi_0 \;=\; (1+n-1)(a^\dagger)^n\varphi_0 \;=\; n(a^\dagger)^n\varphi_0 \tag{1.7}$$

which proves our claim.

The total number operator is sum of all the auxillary operators. That is,

$$\hat{N} \;=\; \sum_{l=1}^{L} n_l \tag{1.8}$$

and thus, the action of the total number operator on a Fock state is

$$\hat{N}|n_1, \ldots, n_L\rangle \;=\; \left(\sum_{l=1}^{L} n_l\right)|n_1, \ldots, n_L\rangle \tag{1.9}$$

□

2 The Fermionic Number Operator

Problem: For a system of fermionic modes, the creation and annihilation operators b_l and $b_l^\dagger$ satisfy the anticommutation relations:

$$\{b_l, b_n^\dagger\} = \delta_{ln}\mathbb{I}, \quad \{b_l, b_n\} = \{b_l^\dagger, b_n^\dagger\} = 0$$

Prove that the number operator $\hat{N} = \sum_{l=1}^{L} b_l^\dagger b_l$ has eigenvalues 0 and 1 for each mode, and show why this implies the Pauli exclusion principle.

Proof. We build on from a similar framework as we did from the Bosonic model. However, the Common Anticomutator Relation(CAR) implies the follwing.

$$\{b_n^\dagger, b_n^\dagger\} \;=\; 2(b_n^\dagger)^2 \;= 0 \quad \text{or} \quad (b^\dagger)^2 \;=\; 0 \tag{2.1}$$

This implies that for Fauk states that have $n_l > 1$, the state must be identically zero.

The pauli exclusion principle states that there cannot be more than one electron in one state, and the CAR implies this principle; if a state had more than one electron in one level, it would be equivalent to the zero state. □

3 Schrodinger and Heisenberg representations

Problem: Suppose A is an observable in the quantum system $\mathcal{S}$. What is the Schrodinger representation and the Heisenberg representation of A? Derive a relation between the two observables.

Solution. The Schrodinger representation of the observable is a time indepen-dant matrix that describes the observable. From the representation, we can derive the expected value of the observable given a state $\Psi(t)$

$$\langle A \rangle \;=\; \langle \Psi(t), A\Psi(t) \rangle \tag{3.1}$$

Suppose the time evolution of $\Psi(t)$ is governed by a time evolution operator $U(t)$, i.e.

$$\Psi(t) \;=\; U(t)\Psi_0 \tag{3.2}$$

where Ψ_0 is the initial state. Then, the expected value of the observable can be rewritten as

$$\langle A \rangle \;=\; \langle U(t)\Psi_0, AU(t)\Psi_0 \rangle \;=\; \langle \Psi_0, U(t)^\dagger AU(t)\Psi(0) \rangle \;=\; \langle U(t)^\dagger AU(t) \rangle_H \tag{3.3}$$

where the time dependence has been incorporated into the observable, not the state. This new time dependent operator is the **Heisenberg Representation** of observable A. In symbols,

$$A(t) \;:=\; U(t)^\dagger AU(t) \tag{3.4}$$

Recall the Schrodinger equation. The time derivative operator is govenred by the Hamiltonian. We assume the Hamilonian to be time independent and self-adjoint.

$$i\frac{\partial}{\partial t}U(t) \;=\; H(t)U(t) \quad \text{and} \quad -i\frac{\partial}{\partial t}U(t)^\dagger \;=\; U(t)^\dagger H(t)^\dagger \tag{3.5}$$

Take the time derivative of equation (3.3) by invoking the chain rule.

$$\begin{aligned}\frac{\partial}{\partial t}A(t) \;&=\; \left(\frac{\partial}{\partial t}U(t)^\dagger\right) AU(t) + U^\dagger(t)A\left(\frac{\partial}{\partial t}U(t)\right) \\ &=\; U(t)^\dagger \left(iH^\dagger A - iAH\right) U(t)\end{aligned} \tag{3.6}$$

Thus,

$$\dot{A}(t) \;=\; [A(t), H(t)] \tag{3.7}$$

where $H(t)$ is the Heisenberg representation of the Hamiltonian.

Also, if the Shrodinger equation is time-dependent, then

$$\dot{A}(t) \;=\; [A(t), H(t)] + i\frac{\partial}{\partial t}A \tag{3.8}$$

□

2.4 Dynamics for a Quantum System: Schrödinger Representation

Problem: Starting from the Schrödinger equation:

$$i\frac{\partial}{\partial t}\Psi(t) = H(t)\Psi(t)$$

derive the expression for the unitary time evolution operator $U(t, t_0)$ when the Hamiltonian $H(t)$ does not explicitly depend on time. Then, generalize this result for the time-dependent case where $[H(t_1), H(t_2)] = 0$ for all t_1, t_2.

Solution. First assume that the Hamiltonian is constant. Then, the equation is separable, and we notice that

$$i\left(\frac{\partial}{\partial t}\Psi(t)\right)\frac{1}{\Psi(t)} \;=\; H \tag{3.9}$$

and by taking the derivative with respect to time both sides,

$$\ln\left(\Psi(t)\right) \;=\; -iHt + \ln(A) \tag{3.10}$$

and thus,

$$\Psi(t) \;=\; Ae^{-iHt} \tag{3.11}$$

where the constant A depends on the initial condition. We know that $\Psi(0)$ is the initial state. Hence,

$$\Psi(t) \;=\; e^{-iHt}\Psi(0) \tag{3.12}$$

Suppose the Hamiltonian varies as a function of time, but the evolution is time independent. That is, for any $t_1, t_2 > 0$,

$$[U(t_1), U(t_2)] \;=\; 0. \tag{3.13}$$

We repeat the process layed below.

$$i\left(\frac{\partial}{\partial t}\Psi(t)\right)\frac{1}{\Psi(t)} = H(t) \tag{3.14}$$

$$\ln(\Psi(t)) - \ln(\Psi(0)) = -i\int_0^t H(u)du \tag{3.15}$$

$$\Psi(t) = \exp\left(-i\int_0^t H(u)du\right)\Psi(0) \tag{3.16}$$

Based on the integral, it is possible to obtain the commutator of two time evolution operators.

$$[U(t_1), U(t_2)] \;=\; \int_0^{t_2}\int_0^{t_1}[H(u), H(v)]dvdu \tag{3.17}$$

So if the Hamilonians-which are also Schrodinger representations, and hence a matrix- do not commute, then it is not guaranteed that

$$U(t_1)U(t_2) \ = \ U(t_2)U(t_1) \tag{3.18}$$

□

2.5 Heisenberg Uncertainty Principle

Problem: Consider two operators A and B acting on a Hilbert space H. The uncertainties ΔA and ΔB are defined as:

$$(\Delta A)^2 = \langle \psi, (A - \langle A \rangle)^2 \psi \rangle, \quad (\Delta B)^2 = \langle \psi, (B - \langle B \rangle)^2 \psi \rangle$$

where $\langle A \rangle = \langle \psi, A\psi \rangle$ and similarly for B. Prove the Heisenberg uncertainty principle:

$$\Delta A \Delta B \geq \frac{1}{2} |\langle [A, B] \rangle|$$

where $[A, B]$ is the commutator of A and B.

Proof. We apply the Cauchy-Schwartz inequality. The inner product of two vectors are less than the product of their respective norms.

$$\langle (A^2 - \langle A \rangle^2)\Psi, (B^2 - \langle B \rangle^2)\Psi \rangle \ \leq \|(A^2 - \langle A \rangle^2)\Psi\|^2 \|(B^2 - \langle B \rangle^2)\Psi\|^2 \tag{3.19}$$

The norm of $(A^2 - \langle A \rangle^2)\Psi$ squared is

$$\|(A^2 - \langle A \rangle^2)\Psi\|^2 \ = \ \langle (A^2 - \langle A \rangle^2)\Psi, (A^2 - \langle A \rangle^2)\Psi \rangle \ = \ (\Delta A)^4. \tag{3.20}$$

Apply the same equation to B and take square root on both sides equation (3.19).

$$\langle (A - \langle A \rangle)\Psi, (B - \langle B \rangle)\Psi \rangle \ \leq (\Delta A \Delta B)^2 \tag{3.21}$$

[1] Concentrate all operators to one side of the norm.

$$\langle \Psi, (A - \langle A \rangle)(B - \langle B \rangle)\Psi \rangle \ \leq (\Delta A \Delta B)^2 \tag{3.22}$$

It is straightforward to verify the follwing equation.

$$\begin{aligned}(A - \langle A \rangle)(B - \langle B \rangle) \ &= \ \frac{(A - \langle A \rangle)(B - \langle B \rangle) + (A - \langle A \rangle)(B - \langle B \rangle)}{2} \\ &\quad + \frac{(A - \langle A \rangle)(B - \langle B \rangle) - (A - \langle A \rangle)(B - \langle B \rangle)}{2}\end{aligned} \tag{3.23}$$

[1] It is straightforward to show that the LHS of this equation squared is the LHS of (3.19)

We call the former operator F and the latter operator C. Notice that $C^\dagger = -C$ so the operator must be purely imaginary. Taking the expected value of both F, C, we verify that

$$\langle (A - \langle A \rangle)(B - \langle B \rangle) \rangle \;=\; \langle \frac{1}{2} \left(\{A, B\} + i[A, B] \right) \rangle \tag{3.24}$$

Finally, we obtain the Heisenberg inequality by ignoring the anticommutator.

$$(\Delta A \Delta B)^2 \;\geq\; |\langle \frac{1}{2} \left(\{A, B\} + i[A, B] \right) \rangle|^2 \;\geq\; \frac{1}{4} \| \langle [A, B] \rangle \|^2 \tag{3.25}$$

$$\Delta A \Delta B \geq \frac{1}{2} \| \langle [A, B] \rangle \| \tag{3.26}$$

□