Summation of Geometry, Topology and Physics

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April 8th 2024

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1 Chapter 1: Quantum Physics

Chapter introducing the reader to path integral quantization.

1.1 Analytical Mechanics

The first section, on analytical mechanics recap topics of mechanics covered in the TCD modules Mechanics & Advanced Classical Mechanics I & II.

The covered topics include Newtonian mechanics, as well as the Lagrangian formalism and the Hamiltonian formalism. The key outcomes of this to be used in quantum mechanics are the Hamiltonian, Poisson brackets, as an introduction to Lie brackets, symmetries and conserved quantities, and phase and configuration spaces.

1.2 Canonical Quantization

1.2.1 Hilbert space, bras and kets

First we must define Hilbert spaces, denoted \mathcal{H} . In QM, a Hilbert space usually means the space of square integrable¹ functions $L^2(M)$ on a space (manifold) M. However we are required to deal with functions with infinite norm. We then use the rigged Hilbert space, which is the extended Hilbert space containing these functions.

$$\mathcal{H} = \{ |\phi\rangle, |\psi\rangle, \dots \} \tag{1}$$

Elements of \mathcal{H} are called **kets** or **ketvectors**. A ket $|a\rangle$ denotes a particular vector in Hilbert-space. A **bra**, or **bra vector**, $\langle \beta |$ denotes a linear map², $\beta : \mathcal{H} \to \mathbb{C}$, mapping each vector in Hilbert space to a number in \mathcal{C} . The action of this linear map $\langle \beta |$ on the vector $|a\rangle$ is then denoted by $\langle \beta | a \rangle \in \mathbb{C}$.

The set of linear functions is also a vector space called the dual vector space of \mathcal{H} . This vector space is denoted by \mathcal{H}^* , and just as kets are elements of \mathcal{H} , bras are elements of \mathcal{H}^* .

We can let the basis of \mathcal{H} be described by $\{e_1, e_2, ...\}$, with the assumptions that \mathcal{H} is separable, and has a countably infinite number of vectors in the basis. This allows us to decompose any $|\psi\rangle$, $|\psi\rangle = \sum_k \psi_k |e_k\rangle$. Similarly we introduce a basis $\{\varepsilon_1, \varepsilon_2, ...\}$ for \mathcal{H}^* which is required to be a dual basis of $\{|e_k\rangle\}$.

Since we can decompose both $|\psi\rangle$ and $\langle\beta|$, the action of $\langle\beta|$ on $|\psi\rangle$ can be written as

$$\langle \beta | \psi \rangle = \sum_{i,j} \beta_i \psi_j \langle \varepsilon_i | e_j \rangle = \sum_{i,j} \beta_i \psi_j \delta_i j = \sum_{i,j} \beta_i \psi_i \tag{2}$$

This can be seen as similar to the product of a vector and a 1-form, producing a scalar.

A one-to-one correspondence can be introduced between \mathcal{H} and \mathcal{H}^* . With fixed bases $\{|e_k\rangle\}$ and $\{\langle \varepsilon_k|\}$, for \mathcal{H} and \mathcal{H}^* respectively, for each $|\psi\rangle = \sum_k \psi_k |e_k\rangle$ there exists a $\langle \psi| = \sum_k \psi_k^* \langle \varepsilon_k| \in \mathcal{H}^*$. It is then possible to define an inner product between two elements $|\phi\rangle$, $|\psi\rangle \in \mathcal{H}$ as

$$(|\phi\rangle, |\psi\rangle) \equiv \langle \phi|\psi\rangle = \sum_{k} \phi_k^* \psi_k. \tag{3}$$

Corresponding bras, kets customarily use the same letter/symbol. From the inner product, we can define the **norm** of a vector $|\psi\rangle$ as

$$\||\psi\rangle\| = \sqrt{\langle\psi|\psi\rangle} \tag{4}$$

easily shown that this satisfies all axioms of the norm, the triangle inequality, absolute homogeneity and positive definiteness. It satisfies positive definiteness due to the complex conjugation of bras.

 $^{^{1}}$ Square integrable functions on space M are those with the integral of the square of their absolute value being finite over M.

²A linear map α is a map with the property of linearity: $\alpha(c_1|\psi_1\rangle+c_2|\psi_2\rangle)=c_1\alpha(|\psi_1\rangle)+c_2\alpha(|\psi_2\rangle) \quad \forall c_i\in\mathbb{C}, |\psi_i\rangle\in\mathcal{H}.$ ³This implies that $\langle \varepsilon_i|e_j\rangle=\delta_{ij}$.

The definition of the inner product allows the construction of an orthonormal basis $\{|e_k\rangle\}$ of \mathcal{H} such that $(|e_i\rangle, |e_j\rangle) = \delta_{i,j}$. It can be shown from the definition of $|\psi\rangle$ that $\langle e_k|\psi\rangle = \psi_k$. This can be inserted into the definition of $|\psi\rangle$ to give $|\psi\rangle = \sum_k |e_k\rangle\langle e_k|\psi\rangle$. Since it is true for all $|\psi\rangle$, this defines the completeness relation

$$\sum_{k} |e_k\rangle\langle e_k| = I \tag{5}$$

where I is the identity operator of \mathcal{H} . (unit matrix when \mathcal{H} is finite dimensional.

1.3 Axioms of Canonical Quantization

For isolated classical dynamical systems, corresponding quantum systems can be constructed following this set of axioms:

- 1. There exists Hilbert space \mathcal{H} for a quantum system, and the state of the system is described by a vector $|\psi\rangle \in \mathcal{H}$. $|\psi\rangle$ is then called the **state** or a **state vector**. Any two states $|\psi\rangle$, $|\phi\rangle$, such that $|\phi\rangle = c \cdot |\psi\rangle$, $c \in \mathbb{C}$, $c \neq 0$, are equivalent, ie. they describe the same state. The state can also be described as a **ray representation** of \mathcal{H} .
- 2. Physical quantity A in CM is replaced by Hermitian operator \hat{A} on \mathcal{H} . Operator \hat{A} is called an **observable**. A measurement of A returns an eigenvalue of \hat{A} . (Hermiticity of \hat{A} assumed to ensure real eigenvalues.)
- 3. PB in CM are replaced by the **commutator** multiplied by $^{-i}/\hbar$ in QM. (Unit in which $\hbar = 1$ assumed from now on.)

$$[\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A} \tag{6}$$

The fundamental commutators analogous to the fundamental PB's are

$$[\hat{q}_i, \hat{q}_j] = [\hat{p}_i, \hat{p}_j] = 0 \quad [\hat{q}_i, \hat{p}_j] = i\delta_{i,j}$$
 (7)

and Hamilton's equation of motion become

$$\frac{\mathrm{d}\hat{q}_i}{\mathrm{d}t} = \frac{1}{i}[\hat{q}_i, \hat{H}] \qquad \frac{\mathrm{d}\hat{p}_i}{\mathrm{d}t} = \frac{1}{i}[\hat{p}_i, \hat{H}] \tag{8}$$

When a classical quantity A is independent of t explicitly, it satisfies the same equation as Hamilton's. Analogously, time-independent \hat{A} satisfies **Heisenberg's equation of motion**

$$\frac{\mathrm{d}\hat{A}}{\mathrm{d}t} = \frac{1}{i}[\hat{A}, \hat{H}] \tag{9}$$

4. Let $|\psi\rangle \in \mathcal{H}$ be an arbitrary state. For many systems in this state, the observation of A at time t returns random results in general. The expectation value of the results is given by

$$\langle A \rangle_t = \frac{\langle \psi | \hat{A}(t) | \psi \rangle}{\langle \psi | \psi \rangle} \tag{10}$$

5. For any physical observable $|\psi\rangle \in \mathcal{H}$, there exists an operator such that $|\psi\rangle$ is one of its eigenstates.

To continue we will examine the 5th axiom. Assuming $|\psi\rangle$ is normalised, suppose $\hat{A}(t)$ has a set of eigenvalues $\{a_n\}$ and corresponding normalised eigenvectors $\{|n\rangle\}^4$, then

$$\hat{A}(t)|n\rangle = a_n|n\rangle \quad \langle n|n\rangle = 1$$
 (11)

Since the eigenvectors are orthonormal, we choose it as the basis and can write arbitrary state $|\psi\rangle$ as

$$|\psi\rangle = \sum_{n} \psi_n |n\rangle \quad \psi_n = \langle n|\psi\rangle$$
 (12)

and the expectation value $\hat{A}(t)$ w.r.t. to $|\psi\rangle$ is

$$\langle \psi | \hat{A}(t) | \psi \rangle = \sum_{m,n} \psi_m^* \psi_n \langle m | \hat{A}(t) | n \rangle = \sum_n |\psi|^2 a_n$$
 (13)

It follows from the fact that the measurement of A in state $|n\rangle$ is always a_n that the probability of the outcome being a_n , ie. that $|\psi\rangle$ is in $|n\rangle$, is

$$|\psi|^2 = |\langle n|\psi\rangle|^2 \tag{14}$$

here the number $\langle n|\psi\rangle$, the weight of state $|n\rangle$ in the state $|\psi\rangle$, is called the **probability amplitude**. For observable \hat{A} with a continuous spectrum a, the state $|\psi\rangle$ is expanded to

$$|\psi\rangle = \int \mathrm{d}a \ \psi(a)|a\rangle \tag{15}$$

and the completeness relation becomes

$$\int \mathrm{d}a \, |a\rangle\langle a| = I \tag{16}$$

Employing the identity returns $\int da' |a'\rangle\langle a'|a\rangle = |a\rangle$, which implies the normalisation

$$\langle a'|a\rangle = \delta(a'-a) \tag{17}$$

the expansion coefficient $\psi(a)$ from Eq.15 is obtained from this normalisation condition as $\psi(a) = \langle a|\psi\rangle$. Since $|\psi\rangle$ is normalised,

$$1 = \int da da' \psi^*(a) \psi(a') \langle a | a' \rangle = \int da |\psi(a)|^2$$
(18)

It follows from Eq. 15 that the expectation value can be defined

$$\langle \psi | \hat{A} | \psi \rangle = \int a |\psi(a)|^2 da$$
 (19)

2 References

⁴Set of eigenvectors can be chosen to be orthonormal due to the hermiticity of $\hat{A}(t)$