Analogy between Classical Canonical Transformations and Quantum Unitary Evolution

Genesis of Path Integral Formulation

IDC412: Seminar Delivery

Aditya Dev

MS19022

Department of Physical Sciences

Indian Institute of Science Education and Research Mohali

Email: ms19022@iisermohali.ac.in

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Contents

Introduction

- Quantum mechanics is built on the analogy with Hamiltonian theory of classical mechanics.
- Canonical coordinates and momenta have simple quantum analogues which allow for the Hamiltonian theory to be transferred into quantum mechanics in all its details.
- There is an alternative formulation for classical dynamics called the Lagrangian method, which is believed to be more fundamental.
- The Lagrangian method allows for all the equations of motion to be expressed as the stationary property of a certain action function, which can be expressed relativistically.

What's the problem then?

- It is not possible to take over the classical Lagrangian equations in a direct way in quantum mechanics as partial derivatives of the Lagrangian with respect to coordinates (*as they are operators in QM*) and velocities have no meaning.
- The only differentiation process that can be carried out in quantum mechanics is that of forming commutation relation, which leads to the Hamiltonian Poission brackets.
- Thus, a quantum Lagrangian theory must be formulated indirectly. The ideas of the classical Lagrangian theory, rather than the equations, must be adopted.

The Hamilton-Jacobi Equation

A **canonical transformation** is a change of canonical coordinates $(q, p, t) \to (Q, P, t)$ that preserves the form of Hamilton's equations. The Action Integral over the Lagrangian $\mathcal{L}_{qp} = \mathbf{p} \cdot \dot{\mathbf{q}} - H(\mathbf{q}, \mathbf{p}, t)$ and $\mathcal{L}_{QP} = \mathbf{P} \cdot \dot{\mathbf{Q}} - K(\mathbf{Q}, \mathbf{P}, t)$ respectively, obtained by the Hamiltonian via ("inverse") Legendre transformation, both must be stationary[1], i.e.

$$\delta \int_{t_1}^{t_2} [\mathbf{p} \cdot \dot{\mathbf{q}} - H(\mathbf{q}, \mathbf{p}, t)]\, dt = \delta \int_{t_1}^{t_2} \left[\mathbf{P} \cdot \dot{\mathbf{Q}} - K(\mathbf{Q}, \mathbf{P}, t)\right] dt = 0 \tag{1}$$

Which implies:

$$p\dot{q} - H = P\dot{Q} - K + \frac{dS}{dt} \tag{2}$$

[1] Canonical transformation. In Wikipedia.

Generating Function and Hamilton's Principal Function

We consider the case when the transformation function S depends on the old and on the new coordinates:

$$S = S(q_1, q_2, \ldots, Q_1, Q_2 \ldots). \tag{3}$$

From Eq 2 and 3, and using Hamiltonian equation of motion, it follows

$$p_r = \frac{\partial S}{\partial q_r}, \quad P_r = -\frac{\partial S}{\partial Q_r} \tag{4}$$

In Hamilton-Jacobi theory where the canonical transformation is such that K is identically zero i.e. $(K = 0)$, it can be shown that[2]:

$$\boxed{S = \int L dt + \text{const.}}, \quad L = \text{Lagrangian} \tag{5}$$

[2] Goldstein, H., Et al. (2001). Classical mechanics third edition. Eq 10.13

Coordinate transformation in Quantum Mechanics

- In the quantum theory we may take a representation in which the q's are diagonal, and a second representation in which the Q's are diagonal.
- The contact (canonical) transformation thus defined corresponds in quantum mechanics to a unitary transformation from the representation in which the quantities q are "diagonal" to the representation in which the quantities Q are "diagonal".
- There will be a transformation function connecting the two representations.

Some Quantum Algebra!!

To find the transformation function let's $\hat{\alpha}$ be a function of dynamical variables in QM, then we may evaluate:

$$\langle q|\hat{A}|Q\rangle = \underbrace{\int dq' \langle q|\hat{A}|q'\rangle \langle q'|Q\rangle}_{\text{Eq 6.1}} = \underbrace{\int dQ' \langle q|Q'\rangle \langle Q'|\hat{A}|Q\rangle}_{\text{Eq 6.2}} \tag{6}$$

We shall now show that this transformation function $\langle q|Q\rangle$ is the quantum analogue of $\mathrm{e}^{iS/\hbar}$

Quantum Theory (cont...)

We know that imposing the commutation relation on position and momentum operator lead to the below equations:

$$[\hat{q}, \hat{p}] = i\hbar \longleftrightarrow \langle q| \hat{p} |\psi\rangle = -i\hbar \frac{\partial \langle q|\psi\rangle}{\partial q} \tag{7}$$

From the definitions in Eq 6.1 we obtain:

$$\langle q| \hat{q}_r |Q\rangle = q_r \langle q|Q\rangle \tag{8}$$

$$\langle q| \hat{p}_r |Q\rangle = -i\hbar \frac{\partial \langle q|Q\rangle}{\partial q_r} \tag{9}$$

similarly from the definitions in Eq 6.2 we obtain:

$$\langle q| \hat{Q}_r |Q\rangle = Q_r \langle q|Q\rangle \tag{10}$$

$$\langle q| \hat{P}_r |Q\rangle = i\hbar \frac{\partial \langle q|Q\rangle}{\partial Q_r} \tag{11}$$

The Postulate!

Now it's turn for **the Postulate!**. In Eq 9 we put:

$$\boxed{\langle q|Q\rangle = e^{iU/\hbar}} \tag{12}$$

where U is a new function of q's and Q's, we get from Eq 9

$$\langle q|\,\hat{p}_r\,|Q\rangle = \frac{\partial U}{\partial q_r}\,\langle q|Q\rangle \tag{13}$$

and similarly from Eq 11, we obtain:

$$\langle q|\,\hat{P}_r\,|Q\rangle = -\frac{\partial U}{\partial Q_r}\,\langle q|Q\rangle \tag{14}$$

Ta Daaa!

Comparing Eq 13 & 14 with Eq 4 we see that:

$$\boxed{p_r = \frac{\partial U}{\partial q_r}, \quad P_r = -\frac{\partial U}{\partial Q_r}} \tag{15}$$

which are exactly like the canonical transformation!!!!
And as shown in Eq 5 the U is nothing but the action; hence we get the familiar transition amplitude as

$$\boxed{\langle q|Q\rangle \sim e^{\frac{i}{\hbar}\int L dt}} \tag{16}$$

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