

Year 2 Quantum Essay

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Research & Writing Methods

For essay 1, I chose to write on self-adjoint operators and their significance when it comes to measurements of real dynamical variables. I have read first few chapters of “The principles of quantum mechanics” by Dirac which is one of the recommended text for this course and found the his explanation on self-adjoint operators really neat.

For essay 2, I chose to write on the hidden variable theory called Bohmian mechanics. Professor Foulkes mentioned hidden variable theories and their limitations a couple of times in his lecture which made me attend the theory group seminar at Imperial given by Antony Valentini where he briefly introduce Bohmian mechanics and his theory of quantum gravity without the Born rule. The talk was based on this paper: [A. Valentini, Beyond the Born rule in quantum gravity, *Found. Phys.* 53, 6 (2023).] I used the references section of the paper to get more information and the references of those references and so on.

Used latex in overleaf for both essays.

1 Reflection on Term 1: Process of Building up Algebra for New Theory

1.1 Principle of Superposition and Indeterminacy

Experimental results require the states of a dynamical system to have the properties of superposition and indeterminacy. The states, therefore can only represent the probability of the outcome of the dynamical variable at time t and can be added to give a new state. This additive nature allow us to assume that *the states are represented as directions of vectors over \mathbb{C}* — often, those vectors live in L^2 , or in general, the Hilbert space of the system.

1.2 Notations and Inner Product

For the purpose of this essay, it suffices to consider that those vectors, which we shall call *kets* (denoted as $|\psi\rangle$), are column vectors and the conjugate transpose (denoted as \dagger) of kets which we call *bras* (denoted as $\langle\psi|$) are row vectors.¹ The notion of norm arises naturally as the inner product of a ket and its corresponding bra:

$$||\psi||^2 = \sum_i |\psi_i|^2 = \sum_i \psi_i^* \psi_i = \boldsymbol{\psi}^\dagger \boldsymbol{\psi} = \langle\psi|\psi\rangle \quad (1)$$

where we also obtained the notion of corresponding bra in matrix representation as $\langle\psi| = \overline{|\psi\rangle} = \boldsymbol{\psi}^\dagger$, overline representing conjugate imaginary.

1.3 Linear Operators

Linear operators act on a function and output another function and satisfy linearity i.e. principle of superposition. This concept is important in quantum mechanics because it is assumed that *the linear operators correspond to the dynamical variables at time t* . By definition, for the algebra of linear operators, the distributive axiom, the associative axiom of multiplication and addition and the commutative axiom of addition hold *but commutativity of multiplication does not hold* which means application of two linear operators on a function, order of the operation matters i.e. in general $TU|\psi\rangle \neq UT|\psi\rangle$.

A linear operator T acting on a bra $\langle\psi|$ is given by $\langle\psi|T$ and is defined as

$$(\langle\psi|T)|\phi\rangle := \langle\psi|(T|\phi\rangle). \quad (2)$$

where $|\phi\rangle$ is an arbitrary ket. Let $\langle A| = \langle\psi|T$, then its conjugate imaginary $\overline{\langle A|}$ depends linearly on $|\psi\rangle$. Thus it is the outcome of some linear operator, which we will denote \overline{T} , on $|\psi\rangle$. \overline{T} is called *adjoint* of T . If kets live in \mathbb{C}^n , then $T : \mathbb{C}^n \rightarrow \mathbb{C}^n$ can be represented as a matrix $T \in M_{n \times n}(\mathbb{C})$. This helps us understanding the adjoint of a linear operators more intuitively. Consider the

¹A ket is a vector in complex Hilbert space H , and a bra is a linear functional $f_\phi : H \rightarrow \mathbb{C}$ in dual vector space H^* , to H where $f_\phi(\psi) := \langle\phi|(\psi) = \langle\phi|\psi\rangle$.

conjugate of inner product between a bra $\langle\psi|T$ and a ket $\bar{T}|\psi\rangle$ which can be expressed as

$$\langle A|\bar{T}|\psi\rangle = \langle\psi|T\bar{T}|\psi\rangle = \overline{\langle A|A\rangle} = \overline{\langle\psi|T\bar{T}|\psi\rangle} = \overline{\langle\psi|T|A\rangle} = \overline{\langle\psi|TA\rangle} = \langle TA|\psi\rangle \quad (3)$$

where $\langle TA|$ is the conjugate imaginary of the result of T operating on $|A\rangle$. In matrix representation, taking the first and the last expression:

$$\langle A|\bar{T}|\psi\rangle = \mathbf{A}^\dagger \bar{\mathbf{T}} \boldsymbol{\psi} = \langle TA|\psi\rangle = (\mathbf{TA})^\dagger \boldsymbol{\psi} = \mathbf{A}^\dagger \mathbf{T}^\dagger \boldsymbol{\psi}. \quad (4)$$

Hence we can conclude that $\bar{T} = \mathbf{T}^\dagger$.

As linear operators we are studying are complex, the dynamical variables corresponding to them must also be complex. We make further assumption that *the adjoint of a linear operator corresponds to the conjugate complex of the dynamical variable*. Therefore, self-adjoint operators (i.e. $T = \bar{T}$) correspond to real dynamical variables. The significance of this will be explained later in terms of measurements and observable quantities.

1.4 Eigenvalues, Eigenvectors and Measurements

Consider the eigenfunction equations with a linear operator T , an arbitrary bra and a ket:

$$T|\psi\rangle = a|\psi\rangle \quad \text{and} \quad \langle\psi|T = b\langle\psi| \quad (5)$$

where $a, b \in \mathbb{C}$. It can be readily shown that if T is self-adjoint, then $a, b \in \mathbb{R}$ and $a = b$ by evaluating $\langle\psi|T|\psi\rangle$ [1]. The solution of the equation (5) is called an eigenstate of the operator T and we say the eigenstate ψ belongs to the eigenvalue a .

We can finally make some assumptions for laws of nature: *if the dynamical system is in an eigenstate of a real dynamical variable T ,² belonging to the eigenvalue a , then a measurement of T will certainly give as result the number a* . Note that a real dynamical variable is chosen instead of a complex one since we expect the result of a measurement to be in \mathbb{R} . *If* a complex dynamical variable were considered as two separate measurements, then it would be either: i) two simultaneous measurements cannot be made or ii) the first measurement would affect the second. This implies that it is not permissible in quantum mechanics. From this assumption, we can infer that if more than one eigenstates belong to the same eigenvalue (degeneracy), then any superposition of them is also an eigenstate belonging to the eigenvalue. Moreover, the eigenvalues are only possible results of a measurement of the real dynamical variable. Conversely, *if more than one eigenstates of a real dynamical variable belong to different eigenvalues, then one state cannot be formed by a linear combination of the others, i.e. orthogonal* — this theorem can be mathematically proven [1].

²Although a dynamical variable T and the corresponding operator T are different, we denote them with the same symbol thanks to the bijection between them.

1.5 Completeness and Probability

First, a couple of assumptions. Physical continuity requires the result of the measurement made at t and $t + dt$ to be the same. Therefore, after measuring, the state *collapses* into the eigenstate belonging to the outcome of the measurement. Furthermore, the state after collapsing on account of a measurement of T , is such that the original state depends on the collapsed state which means, as the original state can be any state, *any state in the Hilbert space of the system can be form by a linear combination of the eigenstates of a real dynamical variable* and such dynamical variables are called *observables*. Surprisingly, another significance of self-adjoint operators is that there exist a theorem stating the converse of our assumption: *for any self-adjoint operator T , there is an orthonormal set of eigenfunctions in which any normalised function can be expanded as a unique linear combination.* [1] Although the theorem is stated without proof,³ considering a case with finite dimensional state space — like we did in chapter 1.3 — provides intuitive understanding of it. Take a state space H whose dimension is finite and a self-adjoint operator T which has a set of eigenvectors $\{v_i\}$. We know for self-adjoint operators that $\langle v_i | v_j \rangle = \delta_{ij}$ and they can be represented as Hermitian matrices (i.e. $T = T^\dagger$) which are diagonalisable, implying $\text{Dim}(H) = |\{v_i\}|$. These two results are sufficient to conclude that $\text{Span}(\{v_i\}) = H$.

In summary, an observable has a corresponding self-adjoint operator T and any physical quantum state $\psi_t(q)$ at time t over a configuration space q can be expressed as

$$\psi_t(q) = \sum_i c_i u_i(q) \quad (6)$$

where u_i is a eigenfunction of T . The complex coefficients c_i of the linear combination are found using

$$c_i = \langle u_i | \psi_t \rangle \quad (7)$$

which is ‘projection of ψ onto basis u_i ’ and are called *probability amplitudes* because of another assumption we make: *The expectation value $\langle T \rangle_{\psi_t}$ of a measurement of observable T in normalised state ψ_t at time t is $\langle \psi_t | T | \psi_t \rangle$.* Consequently, if ψ_t is decomposed into its eigenfunctions u_i , then

$$\langle T \rangle_{\psi_t} = \sum_i c_i \langle \psi_t | T | u_i \rangle = \sum_i c_i a_i \langle \psi_t | u_i \rangle = \sum_i c_i \bar{c}_i a_i \quad (8)$$

where a_i is the eigenvalue to which u_i belongs. Therefore $|c_i|^2$ is interpreted as the probability of measuring a_i . Now, with these physical interpretations and magic equations (5), (6) and (7), we have built up the new way to ‘do physics’, which is to manipulate physical variables i.e. algebra.

³The keywords for googling: self-adjoint operator in infinite dimensional Hilbert space, spectral theory and Hermitian matrices.

2 Extension: Quantum Mechanics as a Limit of More Fundamental Theory

2.1 Probability and Causality

Indeterministic nature of quantum mechanics is the most strangest concept I have ever encountered and the most frustrating limitation of the theory is that we cannot know anything about trajectory of a particle. This-non causal nature⁴ of the theory made me question completeness of it.

One might argue quantum states are the causes but this leads to ‘same cause-different effect’. In contrast, Maxwell distribution, for example, is also a statistical theory (i.e. at given temperature, we know the probability distribution of the speed of a particle rather than its definite speed) but it is justified by Newtonian mechanics (in this theory, the speed can be calculated) at microscopic level. Hidden variable theory is Newtonian mechanics equivalent of quantum theory, asserting *the existence of hidden variables which determine the result of a measurement yet it is not part of quantum mechanics*.

2.2 Bell’s Theorem and Non-Locality

The principle of locality states that a particle is influenced directly only by its immediate surroundings. The alternative to this concept is non-local action at a distance. In 1964, Bell constructed a theorem that states a mechanism such that *the setting of one measuring instrument influences the result of another measurement with a non-local (i.e. instantaneous) propagation of the signal must be involved in a deterministic theory* in which hidden-variables are added to quantum mechanics without changing the statistical predictions. [2]

2.3 De Broglie–Bohm Theory

De Broglie–Bohm theory, also known as the pilot wave theory, is non-local, causal and deterministic. The existence of *actual physical configuration of particles at all times whose evolution over time is determined by the “guiding equation”* in terms of the wavefunction (also known as pilot wave or matter wave) associated with the system of particles, *even when not being measured* — this is the key difference to quantum mechanics — is postulated and the positions of the particles in a system are the “hidden variables” in this theory. [3]

Note that the Born rule (i.e. $\rho = |\psi|^2$) in this theory is not an axiom but the condition for *quantum equilibrium*, which is analogous to classical thermal equilibrium. In Bohm’s papers [3, 4, 5] it was derived from statistical-mechanical methods that asymptotic relaxation from quantum non-equilibrium to quantum equilibrium ($\rho \rightarrow |\psi|^2$) arises as a result of random collisions.

⁴Let alone causality per se has many seemingly unanswerable problems such as: is it an a priori? Even if we assume it is true a priori, we can never *see* the causes (e.g. forces, electric fields, spacetime) and patterns in observation are only things that we can see.

2.3.1 Guiding Equation

The velocity of a particle at time t depends on the guiding equation which is dependent on the configuration of all the particles in the system at t — this makes the theory inherently non-local.

To derive the equation, we assume de Broglie's hypothesis $\mathbf{p} = \hbar \mathbf{k}$ and consider a simple case where the pilot wave is a plane wave: $\psi_t(\mathbf{q}) = |\psi| e^{i(\mathbf{k} \cdot \mathbf{q} - \omega t)}$. In a system with one particles in \mathbb{R}^3 ($\mathbf{q}(t) = x(t)\hat{\mathbf{x}} + y(t)\hat{\mathbf{y}} + z(t)\hat{\mathbf{z}}$), the pilot wave evolves according to the conventional Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \psi = \hat{H} \psi = -\frac{\hbar^2}{2m} \nabla^2 \psi + V \psi \quad (9)$$

where ∇ is over configuration space as usual throughout this essay. [6] As we know that any complex function $\psi_t(\mathbf{q})$ can be written as $R(\mathbf{q}, t) e^{iS(\mathbf{q}, t)}$ where $R, S \in \mathbb{R}$, it is deduced that $\nabla \psi = i\mathbf{k}\psi = (\nabla R/R + i\nabla S)\psi$. Assuming $\mathbf{p} = m(d\mathbf{q}/dt)$, we get the guiding equation

$$\frac{d\mathbf{q}}{dt} = \frac{\hbar}{m} \mathbf{k} = \frac{\hbar}{m} \text{Im} \left(\frac{\nabla \psi}{\psi} \right) = \frac{\hbar}{m} \nabla S. \quad (10)$$

This can be generalised to the individual particle in a system of N particles.

The equations (9) and (10) are adequate to fully describe deterministic dynamics of all the particles in the system with no statistics. [6] For instance, given the initial $\psi_0(\mathbf{q})$, the general solution $\psi_t(\mathbf{q})$ to (9) can be found and given initial position $\mathbf{q}(0)$ and the general $\psi_t(\mathbf{q})$, not only can we find general velocity $\dot{\mathbf{q}}(t)$, integrating (10) gives the general solution for the position $\mathbf{q}(t)$ of the particle.

2.3.2 Statistical Analysis in Terms of Fluid Dynamics

For an ensemble of particles, we may define an actual mass density $\rho(\mathbf{q}, t)$ of configuration \mathbf{q} at time t from which we can derive a continuity equation of the distribution $\rho(\mathbf{q}, t)$. Assuming the conservation of the total mass in the system, self-evidently, the flow of mass coming into an arbitrary volume must be equal to the rate of increase in mass inside the volume. Using the divergence theorem, the continuity equation is

$$\frac{\partial}{\partial t} \iiint_V \rho dV = - \oint_{\mathcal{S}(V)} \rho \dot{\mathbf{q}} \cdot d\mathcal{S} \iff \frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \dot{\mathbf{q}}) \quad (11)$$

where $\dot{\mathbf{q}}(\mathbf{q}, t)$ is velocity field of the distribution and \mathcal{S} is the surface enclosing the arbitrary volume V . [6] From the Schrödinger equation (9), the first derivative of R^2 with respect to t is given by

$$\frac{\partial R^2}{\partial t} = \frac{\partial |\psi|^2}{\partial t} = \frac{i}{\hbar} (\psi (\hat{H} \psi)^* - \psi^* \hat{H} \psi) = -\nabla \cdot \left(R^2 \frac{\hbar}{m} \nabla S \right) = -\nabla \cdot (R^2 \dot{\mathbf{q}}). \quad (12)$$

which implies that *if the initial distribution is in quantum equilibrium, i.e. $\rho(\mathbf{q}, 0) = |\psi_0(\mathbf{q})|^2 = R^2(\mathbf{q}, 0)$, it continues to be in equilibrium at all t .* [6]

Moreover, even if $\rho(\mathbf{q}, 0) \neq |\psi_0(\mathbf{q})|^2$, $\psi_t(\mathbf{q})$ is determined at all t by (9) and ψ_0 which then can be used to obtain the velocity field $\dot{\mathbf{q}}(\mathbf{q}, t)$ at all t by (12). Consequently, integrating (11) gives the entire distribution $\rho(\mathbf{q}, t)$ at all t . [6]

2.3.3 Result: Double Slit Experiment

Electron double slit experiment can be explained in terms of de Broglie–Bohm theory. As we have discussed, individual particle has a well-defined trajectory that passes through one of the slits. Which slit it passes through or which trajectory it takes depend on its initial position. The observer of this experiment, however, cannot know the exact initial condition by physical limitation — it is this lack of knowledge that gives a rise to Heisenberg’s uncertainty principle in de Broglie–Bohm theory [5] — so some degree of randomness is introduced in the pattern detected. Bohm showed that a quantum potential that yields trajectories streaming through the two slits results in interference pattern on the detector screen. [3]

2.4 Conclusion

Double slit experiment is one of the many examples of the consequences of the theory which agree with experiments as *it is supposed to reproduce the results of quantum mechanics by design*. [5] Some (including Einstein and Pauli) argue that the de Broglie–Bohm theory is too contrived. But I believe it is as contrived as all the other theories such as electromagnetism and Newtonian mechanics. When a new fundamental theory is constructed, we “invent” the causes (e.g. forces, fields or energy) of observations and then find/invent a mathematical model that “fits” the patterns in reality up to the highest precision at the time.

Reference

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