Quantum Mechanics

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Abstract

Quantum Mechanics Lecture Notes.

1 Introduction

1.1 Schrödinger formalism

$$\hat{f}\Phi = E\Phi \tag{1.1}$$

$$\Phi \to dP = |\Phi|^2 dq \tag{1.2}$$

$$x \leftrightarrow \hat{x} \tag{1.3}$$

$$p_x \leftrightarrow -i\hbar\frac{\partial}{\partial x} \tag{1.4}$$

$$f \leftrightarrow \hat{f} \tag{1.5}$$

$$\bar{f} = \int \hat{f} dp = \int \Phi^* \hat{f} \Phi dq \tag{1.6}$$

$$[\hat{f}, \hat{g}] = \hat{f}\hat{g} - \hat{g}\hat{f} \tag{1.7}$$

$$\{\hat{f}, \hat{g}\} = \hat{f}\hat{g} + \hat{g}\hat{f} \tag{1.8}$$

1.2 Heisenberg formalism

> Schrödinger was good at math, which is why his quantum mechanics formalism is full of complex mathematical constructs. Heisenberg, on the other hand, had a lot of difficulty with math, which is why his matrix quantum mechanics formalism is limited almost exclusively to linear algebra constructs
>
> Roman ...

Name	Schrödinger	Heisenberg
State Basis	Wave function of basis states $\{\Phi_n\}$	Column vector of basis states $\begin{pmatrix}\phi_1 \\ ... \\ \phi_n\end{pmatrix}$
Observables	Operator $\bar{f} = \int \Phi_n^* \hat{f} \Phi_m$	Operator matrix $\begin{pmatrix}\phi_{11} & ... & \phi_{n1} \\ & ... & \\ \phi_{1n} & ... & \phi_{nn}\end{pmatrix}$
Shrödinger Equation	$\hat{f}\Phi = E\Phi$	$\begin{pmatrix}\phi_{11} & ... & \phi_{n1} \\ & ... & \\ \phi_{1n} & ... & \phi_{nn}\end{pmatrix}\begin{pmatrix}\psi_1 \\ ... \\ \psi_n\end{pmatrix} = \lambda\begin{pmatrix}\psi_1 \\ ... \\ \psi_n\end{pmatrix}$

Building an operator's matrix

For a system with a discrete state basis, $\{\Psi_n\}$, any state of the system can be described as a linear combination of the basis' wave functions:

$$\Psi = \sum_n a_n \Psi_n \tag{1.9}$$

Observable $\bar{f}$ for such a wave function can be decomposed into a sum over the basis state wave functions:

$$\begin{aligned}
\bar{f} &= \int \Psi^* \hat{f} \Psi dq = \int \sum_n a_n^* \Psi_n^* \hat{f} \sum_m a_m \Psi_m dq \\
&= \sum_n \sum_m a_n^* a_m \int \Psi_n^* \hat{f} \Psi_m dq = \sum_n \sum_m a_n^* a_m f_{nm}(t) \\
&= \sum_n \sum_m a_n^* f_{nm}(t) a_m
\end{aligned} \tag{1.10}$$

Where f_{nm} is the operator matrix.

$f_n m(t)$ time dependence

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Solutions to the time-independent Shrödinger equation:

$$\hat{H}\Psi_n = E_n \Psi_n \tag{1.11}$$

$$\Psi_n(t) = e^{-\frac{i}{\hbar}E_n t}\Phi_n \tag{1.12}$$

Which, in operator matrix terms translates into

$$\begin{aligned}
f_{nm}(t) &= \int \Psi_n^* \hat{f} \Psi_m dq = \int \Phi_n^* (e^{-\frac{i}{\hbar}E_n t})^* \hat{f} \Phi_m e^{-\frac{i}{\hbar}E_m t} dq \\
&= e^{+\frac{i}{\hbar}E_n t} e^{-\frac{i}{\hbar}E_m t} \int \Phi_n^* \hat{f} \Phi_m dq = e^{i\frac{E_n - E_m}{\hbar}t} \int \Phi_n^* \hat{f} \Phi_m dq \\
&= f_{nm} e^{i\omega_{nm} t}
\end{aligned} \tag{1.13}$$

Operator matrix properties

1. The operator matrix is hermitian [1] Transposed operator:

$$(\int \Phi \hat{f} \Psi dq \quad)^T = \int \Psi (\hat{f})^T \Phi dq \tag{1.14}$$

   Complex conjugate:

$$(\hat{f})^* = \hat{f}^* \tag{1.15}$$

   Hermitian conjugate:

$$\bar{f}^* = \int \Psi^* \hat{f}^\dagger \Psi dq \tag{1.16}$$

[1] $H^\dagger = H = (H^*)^T$

In operator matrix terms:

$$
\begin{aligned}
(f^*_{nm}) &= \int \varphi^*_n \hat{f}^\dagger \varphi_m dq = \int \varphi^*_n (\hat{f}^*)^T \varphi_m dq \\
&= \int \varphi_m (\hat{f}^* \varphi^*_n) dq = (\int \varphi^*_m \hat{f}^\dagger \varphi_n dq)^* = (f_{mn})^*
\end{aligned} \tag{1.17}
$$

Which means, if f_{nm} is real, meaning $f^*_{nm} = f_{nm}$ that

$$
f_{nm} = f^*_{mn} = f^\dagger_{nm} \tag{1.18}
$$

2. The matrix' diagonal elements are time-independent and real

$$
f_{nn} = \int \Psi_n \hat{f} \Psi_n dq \equiv \bar{f}_n \tag{1.19}
$$

Where $\bar{f}_n$ is the value of observable f in basis state n.

3. The matrix of the product of two operators is the product of their matrices

For operators $\hat{f}$ and $\hat{g}$, what is the operator matrix for operator $\hat{f} \times \hat{g}$ — $(\hat{f} \times \hat{g})_{nm}$?

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$$
\hat{f}\varphi_n = \sum_m f_{mn}\varphi_m \tag{1.20}
$$

$$
\begin{aligned}
\int \varphi^*_k dq \times \hat{f}\varphi_n &= \int \varphi^*_k dq \times \sum_m f_{mn}\varphi_m \\
\int \varphi^*_k \hat{f}\varphi_n dq &= \sum_m f_{mn} \int \varphi^*_k \varphi_m dq f_{kn} = \sum_m f_{mn}\delta_{km} = f_{kn}
\end{aligned} \tag{1.21}
$$

Because for state basis φ_n, φ_n and φ_m are orthogonal for all $m \neq n$.

Using 1.18, we can write:

$$
\begin{aligned}
\hat{f}\hat{g}\varphi_n &= \hat{f}(\hat{g}\varphi_n) = \hat{f}\sum_k g_k n \varphi_k = \sum_k g_{kn}\hat{f}\varphi_k \\
&= \sum_k g_{kn} \sum_m f_{mk}\varphi_m = \sum_{k,m} g_{kn} f_{mk}\varphi_m \\
&= \sum_{k,m} f_{mk} g_{kn}\varphi_m
\end{aligned} \tag{1.22}
$$

And knowing that:

$$
(\hat{f}\hat{g})\varphi_n = \sum_m (\hat{f}\hat{g})_{nm}\varphi_m \tag{1.23}
$$

We end up with:

$$
(\hat{f}\hat{g})_{mn} = \sum_k f_{mk} g_{kn} \tag{1.24}
$$

4. The operator's matrix is equivalent to the operator

$$
\Psi = \sum_m c_m \varphi_m \tag{1.25}
$$

$$\hat{f}\Psi = f\Psi \tag{1.26}$$
$$\hat{f}\sum_m c_m\varphi_m = f\sum_m c_m\varphi_m$$
$$\int \varphi_n^*\hat{f}\sum_m c_m\varphi_m dq = \int \varphi_n^* f\sum_m c_m\varphi_m dq$$
$$\sum_m c_m\int \varphi_n^*\hat{f}\varphi_m dq = f\sum_m c_m\int \varphi_n^*\varphi_m dq$$
$$\sum_m c_m f_{nm} = f\sum_m c_m\delta_{nm}$$
$$\sum_m c_m f_{nm} = f c_n \tag{1.27}$$
$$\tag{1.28}$$

$$\sum_m c_m f_{nm} = f c_n$$
$$\sum_m f_{nm} - f\delta_{nm}c_m = 0 \Rightarrow$$
$$||\ f_{nm} - f\delta_{nm}\ || = 0 \tag{1.29}$$
$$\tag{1.30}$$

1.3 Switching to a different state basis

$\{\varphi_n(q)\}$ and $\{\varphi'_n(q)\}$ are two different basis's.

$$\varphi'_n(q) = \sum_m S_{mn}\varphi_n(q) \tag{1.31}$$
$$\varphi'_n = \hat{S}\varphi_n \tag{1.32}$$

Where $\hat{S}$ is the transition operator. If the new basis$\{\varphi'_n(q)\}$ is orthogonal, meaning:

$$\int \varphi'^*_m\varphi'_n dq = \delta_{mn} \tag{1.33}$$

then $\hat{S}^\dagger = \hat{S}^{-1}$. Proof

$$\sum_l S^*_{lm}S_{ln} = \delta_m n \tag{1.34}$$

Operators in the new basis can be written as:

$$\int \varphi'^*_m\hat{f}\varphi'_n dq = \int (\hat{S}^*\varphi^*_m)(\hat{f}\hat{S}\varphi_n)dq =$$
$$= \int \varphi^*_m\hat{S}^{*T}\hat{f}\hat{S}\varphi_n)dq = \int \varphi^*_m\hat{f}'\varphi_n dq \Rightarrow$$
$$\hat{f}' = \hat{S}^{*T}\hat{f}\hat{S} = \hat{S}^\dagger\hat{f}\hat{S} = \hat{S}^{-1}\hat{f}\hat{S} \tag{1.35}$$

The operator's matrix's trace is the sum of the operator matrix's diagonal elements:

$$Sp\hat{f} = \sum_n f_{nn} \tag{1.36}$$

Proof

1. The trace of the product of two operators is invariant to the order of the operators

$$Sp(\hat{f}\hat{g}) = Sp(\hat{g}\hat{f}) \tag{1.37}$$

2. The trace of the product of three or more operators is invariant to the cyclic permutation of the operators

$$Sp(\hat{f}\hat{g}\hat{h}) = Sp(\hat{h}\hat{f}\hat{g}) = Sp(\hat{g}\hat{h}\hat{f}) \tag{1.38}$$

The operator's matrix's trace is invariant to the basis.

$$Sp\hat{f}' = Sp\hat{S}^{-1}\hat{f}\hat{S} = Sp\hat{S}\hat{S}^{-1}\hat{f} = Sp\hat{f} \tag{1.39}$$

Commutators Two operators commute if and only if they share a set of basis states. Or, in other words, there exist as basis in which they are both diagonal.
If $\hat{f}$ and $\hat{g}$ commute, then:

$$[\hat{f}, \hat{g}] = \hat{f}\hat{g} - \hat{g}\hat{f} = 0 \tag{1.40}$$

Which means that

$$\sum_k f_{mk}g_{kn} = \sum_k g_{mk}f_{kn} \tag{1.41}$$

If $\{\varphi_n\}$ are eigenfunctions of $\hat{f}$, then $f_{nm} \neq 0$ only if $n = m \rightarrow$

$$\begin{aligned} f_{mm}g_{mn} &= g_{mn}f_{nn} \\ g_{mn}(f_{mm} - f_{nn}) &= 0 \end{aligned} \tag{1.42}$$

Meaning that $g_{mn} = 0$ if $m \neq n$

1.4 Pauli uncertainty principle

The Pauli uncertainty principle states that if the operators of two observables do not commute, than we cannot measure both observables with arbitrary precision at the same time. In other words, that to more certain are we about one observable, the more uncertain we are about the other. For example:

$$[\hat{x}, \hat{p_x}] = i\hbar \tag{1.43}$$

$$\Delta x \Delta p_x \geq \hbar \tag{1.44}$$

or, for an exact relation,

$$\sigma_x \sigma_{p_x} \geq \frac{\hbar}{2} \tag{1.45}$$

$$\sigma_x = \sqrt{< \Delta x^2 >} \quad \sigma_{p_x} = \sqrt{< \Delta p_x^2 >} \tag{1.46}$$

$$\tag{1.47}$$

Single-slit electron diffraction

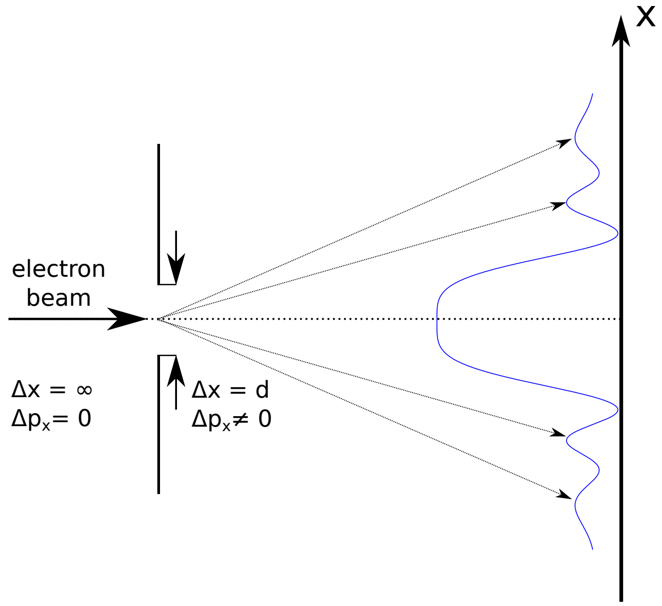

Figure 1.1: Single-slit electron diffraction

$$b\sin(\theta) = \lambda \tag{1.48}$$
$$\Delta p_x = p\sin(\theta) \tag{1.49}$$
$$\Delta x = d \tag{1.50}$$

Using the relation for the de Broglie wavelength

$$\lambda = \frac{h}{p} = \frac{2 * \pi * \hbar}{p} \tag{1.51}$$

We get, considering

$$\Delta x \Delta p_x = d\sin(\theta)\frac{2\pi\hbar}{\lambda} = 2\pi\hbar \tag{1.52}$$
$$\Delta x \Delta p_x \approx \hbar \tag{1.53}$$

Black holes

Quantum Pencil

[1]

1.5 Problems

2 Analytical Solutions

2.1 Rectangular quantum well

2.2 Harmonic oscillator

2.3 Spherically symmetric potential

2.4 Problems

3 Quasi-classical approximation

3.1 Problems

4 Spin

4.1 Problems

5 Perturbation theory

5.1 Time-independent

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6 Problem Solutions

6.1 Introduction

6.2 Analytical solutions

6.3 Quasiclassical approximation

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6.5 Petrubation theory

References

[1] D. Easton, “The quantum mechanical tipping pencil – a caution for physics teachers,” European Journal of Physics, vol. 28, no. 6, p. 1097, 2007.