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Uncertainty Principle and Compatible Operators

The uncertainty of a Hermitian operator on a state of a quantum system vanishes if and only if the state is an eigenstate of the operator. We derive the Heisenberg uncertainty principle, which gives a lower bound for the product of uncertainties of two Hermitian operators. When one of the operators is the Hamiltonian, we are led to energy-time uncertainty relations. The uncertainty inequality is used to derive rigorous lower bounds for the energies of certain ground states. We discuss the diagonalization of operators and prove the spectral theorem, which states that any Hermitian operator or, more generally, any normal operator provides an orthonormal basis of eigenvectors for the state space. We prove that commuting Hermitian operators can be simultaneously diagonalized, addressing the issue of degeneracy. Finally, we discuss complete sets of commuting observables.

15.1 Uncertainty Defined

In quantum mechanics, observables are Hermitian operators. Given one such operator, $\hat{Q}$, we can measure it on a quantum system represented by a state Ψ. If the state Ψ is a $\hat{Q}$ eigenstate, there is no uncertainty in the value of the observable, which coincides with the eigenvalue of $\hat{Q}$ on Ψ. We only have uncertainty in the measured value of $\hat{Q}$ if Ψ is not a $\hat{Q}$ eigenstate but rather a superposition of $\hat{Q}$ eigenstates with different eigenvalues. We gave the definition of uncertainty and its basic properties in section 5.5. In this section we begin with a brief review of the main facts about uncertainty.

Then we discuss a geometric interpretation of the uncertainty in terms of an orthogonal projection.

We call $\Delta Q(\Psi)$ the uncertainty of the Hermitian operator $\hat{Q}$ on the state Ψ. The uncertainty is a nonnegative real number and should vanish if and only if the state is an eigenstate of $\hat{Q}$. Recall that on normalized states Ψ, the expectation value of $\hat{Q}$ is given by

$$\langle \hat{Q} \rangle = \langle \Psi, \hat{Q}\Psi \rangle. \tag{15.1.1}$$

We could write $\langle \hat{Q} \rangle_\Psi$ to emphasize that the expectation value depends on Ψ, but this is usually not done to avoid cluttering the notation. The expectation $\langle \hat{Q} \rangle$ is guaranteed to be a real number since $\hat{Q}$ is Hermitian. We then define the uncertainty $\Delta Q(\Psi)$ as the norm of the vector obtained by acting with $(\hat{Q} - \langle \hat{Q} \rangle \mathbb{1})$ on the state Ψ:

$$\boxed{\Delta Q(\Psi) \equiv \| (\hat{Q} - \langle \hat{Q} \rangle \mathbb{1}) \Psi \|.} \tag{15.1.2}$$

In the above, $\mathbb{1}$ is the identity operator. Defined as a norm, the uncertainty is manifestly nonnegative. We can quickly see that zero uncertainty means the state is an eigenstate of $\hat{Q}$. Indeed, a state of zero norm must be the zero state, and therefore

$$\Delta Q(\Psi) = 0 \;\Rightarrow\; (\hat{Q} - \langle \hat{Q} \rangle \mathbb{1})\Psi = 0 \;\Rightarrow\; \hat{Q}\,\Psi = \langle \hat{Q} \rangle \Psi. \tag{15.1.3}$$

Since $\langle \hat{Q} \rangle$ is a number, the last equation shows that Ψ is an eigenstate of $\hat{Q}$. You should also note that $\langle \hat{Q} \rangle$ is, on general grounds, the eigenvalue. Taking the eigenvalue equation $\hat{Q}\Psi = \lambda\Psi$ and forming the inner product with another Ψ, we get

$$\langle \Psi, \hat{Q}\Psi \rangle = \lambda \langle \Psi, \Psi \rangle = \lambda \quad\Rightarrow\quad \lambda = \langle \hat{Q} \rangle. \tag{15.1.4}$$

Alternatively, if the state Ψ is a $\hat{Q}$ eigenstate, we now know that the eigenvalue is $\langle \hat{Q} \rangle$, and therefore the state $(\hat{Q} - \langle \hat{Q} \rangle \mathbb{1})\Psi$ vanishes, and its norm is zero. We have therefore reconfirmed that the uncertainty $\Delta Q(\Psi)$ vanishes if and only if Ψ is a $\hat{Q}$ eigenstate.

To compute the uncertainty, one usually squares the expression in (15.1.2) so that

$$(\Delta Q(\Psi))^2 = \big\langle (\hat{Q} - \langle \hat{Q} \rangle \mathbb{1})\Psi \,, (\hat{Q} - \langle \hat{Q} \rangle \mathbb{1})\Psi \big\rangle. \tag{15.1.5}$$

One then uses the Hermiticity of the operator $\hat{Q} - \langle \hat{Q} \rangle \mathbb{1}$ to move it from the left entry to the right entry, multiplies out, and evaluates.

Exercise 15.1. *Show that the above steps give the useful expression*

$$(\Delta Q(\Psi))^2 = \langle \hat{Q}^2 \rangle - \langle \hat{Q} \rangle^2, \tag{15.1.6}$$

and conclude that $\langle \hat{Q}^2 \rangle \geq \langle \hat{Q} \rangle^2$.

Geometric interpretation A geometric interpretation of the uncertainty is obtained by thinking about the relation between the states Ψ and $\hat{Q}\Psi$. Let U_Ψ be the one-dimensional vector subspace generated by Ψ. Now consider the state $\hat{Q}\Psi$. If Ψ is not an eigenstate of $\hat{Q}$, the state $\hat{Q}\Psi$ does not lie on U_Ψ. We now claim that

1. the orthogonal projection of $\hat{Q}\Psi$ to U_Ψ is in fact $\langle \hat{Q} \rangle \Psi$,
2. the component of $\hat{Q}\Psi$ in the orthogonal subspace $(\hat{Q} - \langle \hat{Q} \rangle \mathbb{1})$ has a norm equal to ΔQ.

Figure 15.1 shows the various vectors in these claims. To prove (1) and (2), we consider the orthogonal projector P_{U_Ψ} to U_Ψ defined by its action on an arbitrary state η:

$$P_{U_\Psi} \eta = \Psi \, \langle \Psi, \eta \rangle. \tag{15.1.7}$$

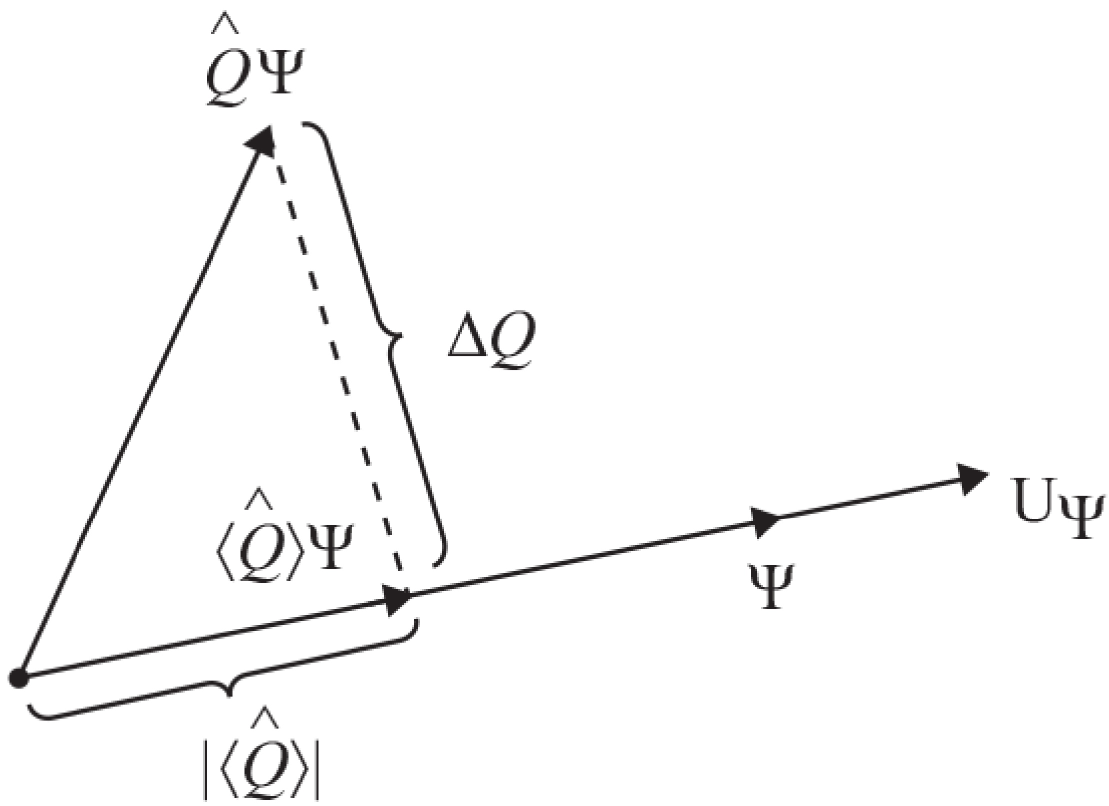

Figure 15.1
A state Ψ and the one-dimensional subspace U_Ψ generated by it. The projection of $\hat{Q}\Psi$ to U_Ψ is $\langle\hat{Q}\rangle\Psi$. The norm of the orthogonal component $(\hat{Q}\Psi)_\perp$ is the uncertainty $\Delta\hat{Q}$.

As it should, the projector leaves invariant any state $c\Psi$ for arbitrary $c \in \mathbb{C}$ and kills any state orthogonal to Ψ. Claim (1) is quickly verified by calculating the projection of $\hat{Q}\Psi$ to U_Ψ:

$$P_{U_\Psi}\hat{Q}\Psi = \Psi\,\langle\Psi, \hat{Q}\Psi\rangle = \Psi\,\langle\hat{Q}\rangle. \tag{15.1.8}$$

Moreover, the vector $\hat{Q}\Psi$ minus its projection to U_Ψ must be a vector $(\hat{Q}\Psi)_\perp$ orthogonal to Ψ:

$$\hat{Q}\Psi - \langle\hat{Q}\rangle\Psi = (\hat{Q}\Psi)_\perp, \tag{15.1.9}$$

as is easily confirmed by taking the inner product with Ψ. Since the norm of the above left-hand side is the uncertainty, we confirm that

$$\Delta Q = \|(\hat{Q}\Psi)_\perp\|, \tag{15.1.10}$$

as claimed in (2). These results are illustrated in figure 15.1. The uncertainty is the shortest distance from $\hat{Q}\Psi$ to the subspace U_Ψ. The magnitude of the expectation value of $\hat{Q}$ is the length of the projection of $\hat{Q}$ Ψ to U_Ψ. Letting χ denote the unit-norm state in the direction of $(\hat{Q}\Psi)_\perp$, we can also write

$$\hat{Q}\Psi = \langle\hat{Q}\rangle\Psi + \Delta Q\,\chi, \quad \langle\chi,\chi\rangle = 1, \quad \langle\chi,\Psi\rangle = 0. \tag{15.1.11}$$

Figure 15.1 makes explicit the Pythagorean relationship:

$$\langle\hat{Q}\rangle^2 + (\Delta Q)^2 = \|\hat{Q}\Psi\|^2, \tag{15.1.12}$$

where the right-hand side is $\langle\hat{Q}\Psi, \hat{Q}\Psi\rangle = \langle\hat{Q}^2\rangle$. This is just (15.1.6).

Example 15.1. *Uncertainty for a linear combination of two different eigenstates.*
Consider two normalized, orthogonal eigenstates ψ_1 and ψ_2 of a linear operator $\hat{Q}$, with eigenvalues q_1 and q_2, respectively:

$$\hat{Q}\psi_1 = q_1\psi_1, \quad \hat{Q}\psi_2 = q_2\psi_2. \tag{15.1.13}$$

Define a normalized state ψ formed as a superposition of the two eigenstates:

$$\psi = \alpha_1\psi_1 + \alpha_2\psi_2, \qquad \alpha_1, \alpha_2 \in \mathbb{C}. \tag{15.1.14}$$

We wish to calculate the uncertainty $\Delta Q(\psi)$ of the operator $\hat{Q}$ in the state ψ.

It is useful to anticipate the answer based on what we know about uncertainty. It is clear that if α_1 vanishes or α_2 vanishes then ψ becomes a $\hat{Q}$ eigenstate, and the uncertainty must vanish. Moreover, if $q_1 = q_2$ the states ψ_1 and ψ_2 are degenerate, and any superposition is an eigenstate of $\hat{Q}$. The uncertainty must vanish in this case as well. All in all, the uncertainty vanishes if $\alpha_1 = 0$, if $\alpha_2 = 0$, and if $q_1 = q_2$. Since the uncertainty has the same units as the operator $\hat{Q}$ and $\hat{Q}$ has the same units as its eigenvalues, we can imagine that $\Delta Q(\psi) \sim \alpha_1\alpha_2(q_2 - q_1)$, an ansatz with the right units that vanishes at the expected values of the parameters. There is one problem, however. The uncertainty must be a nonnegative real number, but the constants α_1 and α_2 are complex numbers, and the difference in eigenvalues could be positive or negative. This can be easily fixed by taking the norm of the complex numbers and the absolute value of the real number:

$$\Delta Q(\psi) \sim |\alpha_1|\,|\alpha_2|\,|q_2 - q_1|. \tag{15.1.15}$$

Let us assume that the above is correct and try to fix the overall constant. For this imagine $\alpha_1 = \alpha_2 = 1/\sqrt{2}$ so that the state $\psi = (\psi_1 + \psi_2)/\sqrt{2}$ is equally likely to be found in the first or in the second state. It follows that the expectation value of $\hat{Q}$ here must be the average of the eigenvalues $(q_1 + q_2)/2$. In the statistical interpretation, the square of the uncertainty is the variance, which is the average of the square of the deviations relative to the mean. But in this case since the mean lies at the midpoint between the possible observed values q_1 and q_2, the absolute value of all deviations is the same and equal to $|q_1 - q_2|/2$. It follows that the variance is this quantity squared, and the standard deviation or uncertainty ΔQ is the quantity $|q_1 - q_2|/2$ itself. This value for ΔQ is predicted by the above formula without any additional multiplicative constant. Thus, the evidence is that

$$\Delta Q(\psi) = |\alpha_1|\,|\alpha_2|\,|q_2 - q_1|. \tag{15.1.16}$$

Let us now confirm this by explicit calculation. Using the orthonormality of ψ_1 and ψ_2 and recalling that ψ is normalized, we have

$$\begin{aligned}
\langle \psi, \psi \rangle &= |\alpha_1|^2 + |\alpha_2|^2 = 1, \\
\langle \psi, \hat{Q}\psi \rangle &= |\alpha_1|^2\, q_1 + |\alpha_2|^2\, q_2, \\
\langle \psi, \hat{Q}^2\psi \rangle &= |\alpha_1|^2\, q_1^2 + |\alpha_2|^2\, q_2^2.
\end{aligned} \tag{15.1.17}$$

It then follows that

$$\begin{aligned}
(\Delta Q(\psi))^2 &= \langle \psi, \hat{Q}^2\psi \rangle - \langle \psi, \hat{Q}\psi \rangle^2 \\
&= |\alpha_1|^2\, q_1^2 + |\alpha_2|^2\, q_2^2 - \left(|\alpha_1|^4\, q_1^2 + |\alpha_2|^4\, q_2^2 + 2|\alpha_1|^2|\alpha_2|^2 q_1 q_2\right) \\
&= q_1^2|\alpha_1|^2(1 - |\alpha_1|^2) + q_2^2|\alpha_2|^2(1 - |\alpha_2|^2) - 2q_1q_2|\alpha_1|^2|\alpha_2|^2 \\
&= (q_1^2 - 2q_1q_2 + q_2^2)|\alpha_1|^2|\alpha_2|^2 \\
&= |\alpha_1|^2|\alpha_2|^2(q_1 - q_2)^2.
\end{aligned} \tag{15.1.18}$$

Taking the square root of this final result, we obtain the claimed (15.1.16). For the generalization of this result to the case of a superposition of multiple orthonormal eigenstates, see problem 15.3.