QUANTUM MECHANICS
Lecture 19

Observables with a continuous spectrum

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D. J. Griffiths: paragraph 3.3

Still about the eigenvectors of a hermitian operator

In the previous lecture, we have concluded that the ***determinate*** states of an observable Q are described by the **eigenvectors** of the self-adjoint (hermitian) operator $\hat{Q}$, representing that particular observable.
We have also said that the opposite is not always true.

Still about the eigenvectors of a hermitian operator

We need, in fact, to distinguish **two cases:**

- the spectrum of $\hat{Q}$ is ***discrete***, which means that the eigenvalues are separated one another;
- the spectrum of $\hat{Q}$ is ***continuous***, which means that the eigenvalues fill some real range.

Still about the eigenvectors of a hermitian operator

1. In the case of ***discrete spectrum***, the **eigenvectors** (eigenfunctions) **can be normalized** and **they belong to the Hilbert space.**

2. According to the postulates of QM, **each of them represents a physical state** which is a **determinate state** for the observable that we are considering.

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Discrete spectrum

Let us remark also that

1. Since the operator representing the observable is self-adjoint, the eigenvalues are real (which is true also in case of continuous spectrum ...).

2. The eigenvectors (eigenfunctions) corresponding to different eigenvalues are mutually orthogonal, in fact

$$< \psi_1|\hat{Q}\psi_2 >=< \hat{Q}\psi_1|\psi_2 >$$
$$\Rightarrow q_2 < \psi_1|\psi_2 >= q_1 < \Psi_1|\psi_2 >\Rightarrow< \psi_1|\psi_2 >= 0$$

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1. This is why **stationary states** corresponding, for instance, to **different energies are orthogonal:** they are eigenfunctions corresponding to different eigenvalues.

2. If an eigenvalue is degenerate, we cannot say anything about the scalar product of two independent eigenvectors corresponding to the **same** eigenvalue.

3. However, there exists a well-defined procedure to find an **orthonormal basis** of the linear subspace made by the eigenvectors corresponding to the same eigenvalue (Gram-Schmidt procedure).

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2. This happens, for instance, in case of finite-dimensional Hilbert spaces, where the spectrum of any operator can only be discrete.

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Discrete spectrum

1. This property for which, given a generic hermitian operator, we can always find an orthonormal basis of the Hilbert space which is made by its eigenvectors, **does not generalize** to infinite-dimensional spaces.

2. However, following Dirac, we will **assume** that **every observable** has this property.

3. The reason is physical. If we measure that particular observable $\hat{Q}$ on any physical state, we will obtain a determinate state of $\hat{Q}$, which means that any state must be a linear combination of such states.

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Discrete spectrum

1. In other words, every hermitian operator representing a **physical observable** and having a **discrete spectrum**, has the eigenvectors that form **a complete set** and, therefore, **any vector belonging to the Hilbert space can be expressed as a linear combination of them.**

2. Moreover, thanks to the Gram-Schmidt orthonormalization procedure, starting from the above complete set, we can always define an **orthonormal basis of eigenvectors.**

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Discrete spectrum

1. This means that if $\hat{Q}$ is an observable with a **discrete, non-degenerate spectrum**, then, in the Hilbert space of the physical states, we can define an orthonormal basis $\{\mathbf{e}(q_j)\}$ made by the eigenvectors of $\hat{Q}$ corresponding to the eigenvalues q_j.
Therefore, a generic physical state described by the vector $\mathbf{v}$ can be written as

$$\mathbf{v} = \sum_j c_j \, \mathbf{e}(q_j) \quad where \quad c_j \equiv < \mathbf{e}(q_j)|\mathbf{v} >$$

2. If we measure the observable $\hat{Q}$ on the state $\mathbf{v}$, the only possible outcome is an eigenvalue of $\hat{Q}$ and the probability to obtain a particular value q_k is $|c_k|^2 = | < \mathbf{e}(q_k)|\mathbf{v} > |^2$.

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Discrete spectrum

1. But what happens if the spectrum of the observable $\hat{Q}$ is discrete, but degenerate ?

2. Also in this case, as we have already said, we can define an orthonormal basis made by eigenvectors (determinate states) of $\hat{Q}$, but, now, **the eigenvalues q_j are not enough to label these vectors, because of the degeneracy.**

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Discrete spectrum

Let us write this orthonormal basis as $\{\mathbf{e}(q_j, k)\}$, where the parameter k is introduced to distinguish the eigenvectors of $\hat{Q}$ corresponding to the same eigenvalue. By definition we have

$$\hat{Q}\,\mathbf{e}(q_j, k) = q_j\;\mathbf{e}(q_j, k)$$

$$< \mathbf{e}(q_i, k_1)|\mathbf{e}(q_j), k_2 >= 0 \quad if \quad q_i \neq q_j$$

$$< \mathbf{e}(q_i, k_1)|\mathbf{e}(q_i), k_2 >= \delta_{k_1 k_2}$$

Discrete spectrum

1. The generic state described by the vector $\mathbf{v}$ can now be represented in this basis as

$$\mathbf{v} = \sum_{q_j,k} c(q_j,k)\ \mathbf{e}(q_j,k), \quad \textit{with}$$
$$c(q_j,k) = < \mathbf{e}(q_j,k)|\mathbf{v} >$$

2. A measurement of $\hat{Q}$ will result again only in an eigenvalue q_s of $\hat{Q}$, but, because of the degeneracy, the probability of measuring such a value (if there are no conditions on k) is now

$$\sum_k |c(q_s,k)|^2$$

because all the states $\mathbf{e}(q_s,k)$, no matter what k is, can contribute !

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Continuous spectrum

1. In case of a *continuous spectrum*, the eigenvectors **do not belong** to the Hilbert space because they **cannot be normalized.**
2. However, we accept them as possible *generalized eigenvectors* if they have **a finite scalar product with any function** (vector) of the Hilbert space.
3. Realizable **physical states** (normalizable) **can only be linear combinations** (wave packets) of these *generalized* eigenvectors, **corresponding to different eigenvalues.**
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1. This is the case, for instance, of the momentum operator $\hat{p} = -i\hbar \frac{d}{dx}$.
2. An eigenfunction of $\hat{p}$ for the eigenvalue p should satisfy the equation

$$\hat{p}\,\psi_p(x) = p\,\psi_p(x) \;\Rightarrow\; -i\hbar\frac{d\psi_p}{dx} = p\,\psi_p$$

$$\Rightarrow \psi_p(x) = A\,e^{ipx/\hbar}$$

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1. **This implies that we cannot realize physical states with a perfectly definite momentum !**

2. However, we accept these functions as **generalized eigenvectors** because, although they cannot be normalized, they have a finite scalar product with **any** square-integrable function ψ *(Dirac condition)*,

$$\int dx\, \psi^*(x)\, \psi_p(x) = A \int dx\, \psi^*(x)\, e^{ipx/\hbar} = c(p) \in C$$

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Normalization

1. Coming to the **normalization** of these functions, let's start by remembering that

$$\int dx\, e^{i\eta x} = 2\pi\, \delta(x)$$

2. therefore, if we define the normalization constant of ψ_p in such a way that

$$\psi_p(x) \equiv \frac{1}{\sqrt{2\pi\hbar}}\, e^{ipx}$$

the momentum generalized eigenfunctions satisfy the **Dirac orthonormality condition**

$$\int dx\, \psi_p^*(x)\, \psi_q(x) = \frac{1}{2\pi\hbar} \int dx\, e^{ix(q-p)/\hbar} =$$

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1. The set $\{\psi_p(x); p \in R\}$ of these eigenfunctions form an **orthonormal, generalized complete set**.
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Continuous spectrum

Let us consider a generic normalized wave function $\psi(x)$.
In case of a finite or numerable orthonormal basis ψ_n, we already know that

$$\psi(x) = \sum_n c_n \, \psi_n(x)$$

where the complex coefficients c_n are the scalar product of the functions ψ_n with ψ:

$$c_n \equiv < \psi_n | \psi > = \int dx \, \psi_n^*(x) \, \psi(x)$$

and one has

$$1 = \int dx \, |\psi(x)|^2 = \sum_n |c_n|^2$$

Continuous spectrum

1. Let us consider, now, the momentum eigenfunctions $\psi_p(x)$. We know that they are orthonormal in the Dirac sense. If, in close analogy to the numerable case, we define

$$
\begin{aligned}
c(p) \equiv \tilde{\psi}(p) &= <\psi_p|\psi>= \int dx\, \psi_p^*(x)\psi(x) = \\
&= \frac{1}{\sqrt{2\pi\hbar}} \int dx\, e^{-ipx/\hbar}\psi(x)
\end{aligned}
$$

2. the Fourier transform theory guarantees that

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\psi(x) &= \int dp\; c(p)\, \psi_p(x) \equiv \int dp\; \tilde{\psi}(p)\, \psi_p(x) \\
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2. the Fourier transform theory guarantees that

$$\psi(x) = \int dp\; c(p)\, \psi_p(x) \equiv \int dp\; \tilde{\psi}(p)\, \psi_p(x) \\ 1 = \int dx\, |\psi(x)|^2 = \int dp\, |\tilde{\psi}(x)|^2$$

About the Fourier transform

In fact, the Fourier transform theory states that, if $f(x)$ is a continuous integrable function, then we can define its Fourier transform $\hat{f}(k)$ as follows

$$\hat{f}(k) = \frac{1}{\sqrt{2\pi}} \int dx\, f(x)\, e^{-ikx}$$

and the ***inverse*** Fourier transform of $\hat{f}(k)$

$$\frac{1}{\sqrt{2\pi}} \int dk\, \hat{f}(k)\, e^{ikx}$$

gives back the original function $f(x)$

$$f(x) = \frac{1}{\sqrt{2\pi}} \int dk\, \hat{f}(k)\, e^{ikx}$$

Continuous spectrum

It is easy, now, to verify that $\tilde{\psi}(p)$ is simply proportional to the Fourier transform $\hat{\psi}(k)$ of the w.f. $\psi(x)$, evaluated in $k = p/\hbar$: in fact

$$\tilde{\psi}(p) \equiv \frac{1}{\sqrt{2\pi\hbar}} \int dx\, e^{-ipx/\hbar} \psi(x) = \\ = \frac{1}{\sqrt{\hbar}}\, \hat{\psi}\left(\frac{p}{\hbar}\right)$$

and, **because of the inverse Fourier transform theorem, we have indeed that**

$$\int dp\, \tilde{\psi}(p)\, \psi_p(x) = \int dp\, \frac{1}{\sqrt{\hbar}}\, \hat{\psi}\left(\frac{p}{\hbar}\right) \frac{1}{\sqrt{2\pi\hbar}}\, e^{ipx/\hbar} = \\ = \frac{1}{\sqrt{2\pi}} \int \frac{dp}{\hbar}\, \hat{\psi}\left(\frac{p}{\hbar}\right)\, e^{ix\frac{p}{\hbar}} = \frac{1}{\sqrt{2\pi}} \int dk\, \hat{\psi}(k) e^{ikx} = \\ = \psi(x)$$