QUANTUM MECHANICS
Lecture 18

Hermitian and Unitary operators
Determinate states
Eigenfunctions and eigenvalues

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D. J. Griffiths: paragraphs 3.3

Exercise N.6

Exercise

In a bidimensional Hilbert space, $\mathbf{e}_1$ and $\mathbf{e}_2$ form an orthonormal basis.

- Consider the system of the two vectors $\mathbf{a}_1 \equiv \mathbf{e}_1 + i\,\mathbf{e}_2$ and $\mathbf{a}_2 \equiv i\,\mathbf{e}_1 - \mathbf{e}_2$.
  Do $\mathbf{a}_1$ and $\mathbf{a}_2$ form a basis ? Explain.
- Show that

$$\mathbf{f}_1 = \frac{1}{\sqrt{2}}(\mathbf{e}_1 + \mathbf{e}_2); \quad \mathbf{f}_2 = \frac{1}{\sqrt{2}}(\mathbf{e}_1 - \mathbf{e}_2)$$

  form an orthonormal basis.
- Write the 2×2 matrix $\mathbf{A}$ that allow to express the vectors $\mathbf{f}_i$ in terms of the vectors $\mathbf{e}_j$, i.e. $\mathbf{f}_i = \mathbf{A}_{ji}\mathbf{e}_j$; $i, j = 1, 2$.

Hermitian operators

1. We have seen that, in a basis $\{\mathbf{e}_j\}$, the linear operator $\hat{Q}$ is completely determined by the square matrix $Q_{kj} \equiv < \mathbf{e}_k | \hat{Q} \mathbf{e}_j >$ such that

$$\hat{Q}\mathbf{e}_j = Q_{kj}\mathbf{e}_k$$

2. To every linear operator $\hat{Q}$ we can associate its **adjoint** $\hat{Q}^\dagger$ by the following definition

$$\forall \mathbf{a}, \mathbf{b} \in \mathcal{H} : < \mathbf{a} | \hat{Q}^\dagger \mathbf{b} > \equiv < \hat{Q}\mathbf{a} | \mathbf{b} >$$

3. The matrix $(Q^\dagger)_{kj}$, describing the operator $\hat{Q}^\dagger$ in the basis $\{\mathbf{e}_j\}$, by definition, is given by

$$\hat{Q}^\dagger \mathbf{e}_j \equiv (Q^\dagger)_{kj}\, \mathbf{e}_k, \quad \mathit{with} \quad (Q^\dagger)_{kj} = < \mathbf{e}_k | \hat{Q}^\dagger \mathbf{e}_j >$$

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$$= (Q^+)_{kj}$$

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which means that the **expectation value** of a self-adjoint operator $\hat{A}$, evalutated on any vector **a**, **is a real quantity**.

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Hermitian operators and physical observables

Since the condition of having a real expectation value on any vector **is a sufficient condition to conclude that the operator is hermitian,**

***we can affirm that the physical observables must be represented by hermitian operators*.**

Hermitian operators and physical observables

This is the reason why every physical observable $\hat{Q} = \hat{Q}(x, -i\hbar\frac{\partial}{\partial x})$, acting on the wave-functions, is such that

$$< \Psi_1|\hat{Q}\Psi_2 > \equiv \int dx\, \Psi_1^*(x,t)\left(\hat{Q}\Psi_2\right)(x,t) =$$

$$= \int dx\, \left(\hat{Q}\Psi_1^*\right)(x,t)\,\Psi_2(x,t) \equiv < \hat{Q}\Psi_1|\Psi_2 >$$

Unitary Operators

1. Another important class of linear operators are the **unitary operators**.
2. The **linear operator** $\hat{U}$ is **unitary** iff

$$\hat{U}\,\hat{U}^\dagger = I = \hat{U}^\dagger\,\hat{U} \quad \Leftrightarrow \quad \hat{U}^\dagger = \hat{U}^{-1}$$

3. These operators are such that

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1. If $\hat{U}$ is unitary, then the matrix U representing the linear operator $\hat{U}$ in a basis $\{\mathbf{e}_j\}$ is also unitary ($\Rightarrow UU^+ = I$); in fact

$$\delta_{kj} =< \mathbf{e}_k|\mathbf{e}_j >=< \hat{U}\mathbf{e}_k|\hat{U}\mathbf{e}_j >=< U_{sk}\mathbf{e}_s|U_{tj}\mathbf{e}_t >=$$
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Determinate states

1. As we already know, in QM, when we measure a physical observable $\hat{Q}$ on a state $\boldsymbol{\Psi}$, usually **we can only predict the probability of obtaining a specific value q.**

2. **Can we realize a physical state**, such that **the measurement** of the observable $\hat{Q}$ **gives, with certainty**, some suitable **real value q ?**

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1. This must be possible, because we know that, if we start from a state $\mathbf{\Psi}_{in}$, we measure $\hat{Q}$ and we obtain some value q, then, if we measure again $\hat{Q}$ on the new physical state $\mathbf{\Psi}_q$ in which the previous one has collapsed after the first measurement, we obtain again the value q.

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Determinate states

1. Which are the characteristics of the (normalized) vector $\mathbf{\Psi}_q$, representing such a ***determinate* state ?**

2. Clearly, the **expectation value** of the operator $\hat{Q}$ (representing the observable Q) evaluated on $\mathbf{\Psi}_q$ **is equal to** q, since every measurement of $\hat{Q}$ performed on the state represented by $\mathbf{\Psi}_q$ has only q as possible outcome:

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1. But since there is only one possible outcome from the measurement, the standard deviation of the probability distribution defined by $|\mathbf{\Psi}_q|^2$ is equal to zero:

$$\sigma_q^2 =< \mathbf{\Psi}_q| \left(\hat{Q}- < Q >\right)^2 \mathbf{\Psi}_q >= 0$$

2. However, $\hat{Q}$ is hermitian and the same is true for $\hat{Q}- < Q >\equiv \hat{Q} - q$ since q is real, therefore

$$0=< \mathbf{\Psi}_q|(\hat{Q} - q)^2\mathbf{\Psi}_q >=< (\hat{Q} - q)\mathbf{\Psi}_q|(\hat{Q} - q)\mathbf{\Psi}_q >=$$
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The equation

$$\hat{Q}\boldsymbol{\Psi}_q = q\,\boldsymbol{\Psi}_q \quad with \quad \boldsymbol{\Psi}_q \neq \mathbf{0}$$

is called the ***eigenvalue equation*** for the operator $\hat{Q}$ and $\boldsymbol{\Psi}_q$ is an **eigenfunction (eigenvector)** of $\hat{Q}$, corresponding to the **eigenvalue** q.

Determinate states

1. Now, **be very careful**.

2. A frequent mistake is to think that, when you measure a physical observable $\hat{Q}$ on a physical state described by the (normalized) vector $\mathbf{\Psi}$, the vector originated after the measurement is $\hat{Q}\mathbf{\Psi}$.

3. **This is false !**

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If and only if $\mathbf{\Psi}$ **is an eigenvector** of the operator $\hat{Q}$ for some eigenvalue q, we have

$$\hat{Q}\mathbf{\Psi} = q\,\mathbf{\Psi}$$

But, also in this case, **it is not true** that the vector describing **the physical state** after the measurement of $\hat{Q}$ is $q\,\mathbf{\Psi}$, but it **remains $\mathbf{\Psi}$.**

Eigenfunctions and eigenvalues

Let us observe, now, that

1. If $\boldsymbol{\Psi}$ is an eigenvector of $\hat{Q}$ for the eigenvalue q, then also $\alpha\,\boldsymbol{\Psi}$ (with $\alpha \neq 0$ ...) has the same property.
2. It may happen that, for a given eigenvalue q, there are **two or more linearly independent eigenvectors.**
3. In this case, **any linear combination of these eigenvectors is an eigenvector** of $\hat{Q}$ for the eigenvalue q and we say that the eigenvalue q is ***degenerate.***
4. The set of all the eigenvalues of the hermitian operator $\hat{Q}$ is its ***spectrum.***

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Eigenfunctions and eigenvalues

Before entering in more general details, let us recall some conclusions that we have already drawn concerning the solution of an "ante-litteram" eigenvalue problem, the time-independent Schrödinger equation

$$\widehat{H}\Psi = E\,\Psi$$

where

- $\widehat{H}$ is the hamiltonian operator;
- E the energy eigenvalue;
- ψ the corresponding eigenvector (eigenfunction).

Eigenfunctions and eigenvalues

1. In the case, for instance, of the **harmonic oscillator**, the energy spectrum is

$$\left\{ E_n = \left(n + \frac{1}{2}\right) \hbar\omega; \;\; n = 0,\, 1,\, \ldots \right\}$$

2. The corresponding normalized eigenfunctions are

$$\psi_n(x) = \left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2^n\, n!}} e^{-\frac{1}{2}\frac{m\omega}{\hbar} x^2} \; H_n\left(x\sqrt{\frac{m\omega}{\hbar}}\right)$$

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Eigenfunctions and eigenvalues

1. As another example, we can consider the hamiltonian $\widehat{H}$ associated to the **infinite square well** between 0 and $+a$.
In this case, the spectrum of $\widehat{H}$ is

$$\left\{ E_n = \frac{\hbar^2}{2m} \left(\frac{n\pi}{a} \right)^2 ; \;\; n = 1, 2, \ldots . \right\}$$

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Still about the eigenvectors of a hermitian operator

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