QUANTUM MECHANICS Lecture 17

Linear Operators in $\mathcal{H}$ and Physical Observables

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D. J. Griffiths: paragraphs 3.2

Hilbert space

In the previous lecture, we have seen that, if $\{\mathbf{e_j}\}$ and $\{\mathbf{f_k}\}$ are two orthonormal bases of a Hilbert space, then there exist two square matrices A and B such that[1]

$$\mathbf{f_k} = A_{jk}\,\mathbf{e_j}; \qquad \mathbf{e_j} = B_{kj}\,\mathbf{f_k}$$

with $A\,B = I$; $\quad (\Rightarrow A = B^{-1};\;\; B = A^{-1})$.

[1] We are using the Einstein convention for which, when an index appears twice, it implies summation of that index over all its possible values.

Hilbert space

1. The matrices A and B describe also the **effect** of the **basis change** on the **components** of a generic vector.
2. In fact, if the components of a generic vector $\mathbf{v}$ in the basis $\{\mathbf{e_j}\}$ are $\{\alpha_j\}$ and in the basis $\{\mathbf{f_k}\}$ are $\{\beta_k\}$, then

$$\mathbf{v} \equiv \alpha_j \mathbf{e_j} = \alpha_j B_{kj} \mathbf{f_k} \equiv \beta_k \mathbf{f_k} \quad \Rightarrow$$
$$\Rightarrow \beta_k = B_{kj} \alpha_j$$

$$\mathbf{v} \equiv \beta_k \mathbf{f_k} = \beta_k A_{jk} \mathbf{e_j} \equiv \alpha_j \mathbf{e_j} \quad \Rightarrow$$
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where we have used the fact that, in a basis, **the components of a vector are unique.**

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1. It can be shown that the linear space of the square-integrable functions $\psi(x)$ **is** a Hilbert space with the following scalar product

$$< \psi_1 | \psi_2 > \equiv \int dx\ \psi_1(x)^* \, \psi_2(x)$$

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According to what we have seen, if $\{\psi_j\}$ is an orthonormal basis of the Hilbert space $\mathcal{H}$ of the square integrable functions in one real variable, then

1. $$< \psi_i | \psi_j > \equiv \int dx \; \psi_i(x)^* \, \psi_j(x) = \delta_{ij}$$

2. if $\psi \in \mathcal{H}$
$$\psi = \sum_j < \psi_j | \psi > \; \psi_j \equiv c_j \, \psi_j$$
where
$$c_j = \int dx \, \psi_j(x)^* \, \psi(x)$$

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Operators and Observables

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2. If the **appropriate mathematical structure** in which to describe the **states of a physical system** in QM is the **Hilbert space**, **which is the corresponding description of the physical observables ?**

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Operators and Observables

1. We have already seen that, to evaluate, for instance, the expectation value of a physical observable $Q = Q(x,p)$ on a physical state described by the w.f. $\Psi(x,t)$, we need to calculate the integral

$$\int dx\, \Psi(x,t)^* \left[\hat{Q}\left(x, -i\hbar\frac{\partial}{\partial x}\right)\, \Psi(x,t)\right]$$

in which we can now recognize the **scalar product** of Ψ and $\hat{Q}\Psi$, being $\hat{Q}$ a **linear operator.**

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2. **But, which is the proper definition of a linear operator in a Hilbert space ?**

Linear operators in a Hilbert space

1. In general, a linear operator $\hat{Q}$ acting on the vectors of a Hilbert space must be such that
   - $\forall \mathbf{a} \in \mathcal{H}$, $\hat{Q}\mathbf{a} \in \mathcal{H}$
   - $\hat{Q}(\mathbf{a} + \mathbf{b}) = \hat{Q}\mathbf{a} + \hat{Q}\mathbf{b}$
   - $\hat{Q}(\alpha\mathbf{a}) = \alpha\,\hat{Q}\mathbf{a}$

2. We have seen that, once we have choosen an orthonormal basis $\{\mathbf{e_i}\}$, **a vector is completely determined by its numerical (complex) components.**

3. **Do we have something similar for a linear operator ?**

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Let us consider an operator $\hat{Q}$ and a generic vector $\mathbf{a} = \alpha_i \mathbf{e}_i$, where $\{\mathbf{e}_i\}$ is a suitable orthonormal basis. We have

$$\hat{Q}\mathbf{a} = \hat{Q}(\alpha_i \mathbf{e}_i) = \alpha_i \, \hat{Q}\mathbf{e}_i$$

But, for any vector $\mathbf{e}_i$ of the basis, we will have

$$\hat{Q}\mathbf{e}_i = Q_{ji}\mathbf{e}_j \;\; where \;\; Q_{ji} =< \mathbf{e}_j|\hat{Q}\mathbf{e}_i > \in C$$

and therefore

$$\hat{Q}\mathbf{a} = \alpha_i \, \hat{Q}\mathbf{e}_i = \alpha_i \, Q_{ji}\mathbf{e}_j = (Q_{ji}\alpha_i)\mathbf{e}_j \;\; \Rightarrow$$
$$\Rightarrow < \mathbf{e}_j|\hat{Q}\mathbf{a} >= Q_{ji}\alpha_i = Q_{ji} < \mathbf{e}_i|\mathbf{a} >$$

Linear operators in a Hilbert space

1. In conclusion, in a given basis $\{\mathbf{e}_i\}$, the action of a linear operator $\hat{Q}$ is described by a suitable complex matrix $Q_{ji} =< \mathbf{e}_j|\hat{Q}\mathbf{e}_i >$, such that the components of a generic vector $\hat{Q}\mathbf{a}$ are given by

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where the $\{\alpha_i\}$ are the component of the vector $\mathbf{a}$, in the same basis.

2. **Let us see, now, what happens to the matrix Q_{ji}, representing a given linear operator $\hat{Q}$, when we change the vector basis.**

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then, if **a** is a generic vector such that

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2. Let

$$< \mathbf{e}_j|\hat{Q}\mathbf{a} >\equiv Q_{ji}\alpha_i$$

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1. Therefore

$$< \mathbf{f}_k|\hat{Q}\mathbf{a} >= \tilde{Q}_{kt}\beta_t = \tilde{Q}_{kt}A^{-1}_{tj}\alpha_j \equiv \left(\tilde{Q}\, A^{-1}\right)_{kj}\, \alpha_j$$

2. On the other hand

$$< \mathbf{f}_k|\hat{Q}\mathbf{a} >=< A_{ik}\mathbf{e}_i|\hat{Q}\mathbf{a} >= A^*_{ik} < \mathbf{e}_i|\hat{Q}\mathbf{a} >=$$

$$= \; A^*_{ik}Q_{ij}\alpha_j = A^+_{ki}Q_{ij}\alpha_j = \left(A^+\, Q\right)_{kj}\, \alpha_j$$

where the matrix $A^+ \equiv (A^t)^*$ is the transposed complex conjugate of the matrix A, called ***the hermitian conjugate*** of A.

3. Given of the arbitrarity of the α_j, we can conclude that it must be

$$\tilde{Q}\, A^{-1} = A^+\, Q \quad \Leftrightarrow \quad \tilde{Q} = A^+\, Q\, A$$

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