Theoretical Physics II B – Quantum Mechanics

Lecture 5

Frank Krauss

February 11, 2014

Solutions to previous control questions

4.1 Determine first the transformation matrix $\hat{T}$ through

$$(\hat{T})_{ij} = \langle\psi_i|\phi_j\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

Since all entries are real and because $\hat{T}$ is symmetric, it is self-adjoint: $\hat{T} = \hat{T}^\dagger$. Therefore

$$\begin{aligned}\hat{A}\Big|_\phi &= \hat{T}^\dagger\ \hat{A}\Big|_\psi\ \hat{T} \\ &= \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} 1 & \epsilon \\ \epsilon & 1 \end{pmatrix}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \begin{pmatrix} 1+\epsilon & 0 \\ 0 & 1-\epsilon \end{pmatrix}.\end{aligned}$$

Note: Realising that the $|\phi_{1,2}\rangle$ are the eigenvectors of $\hat{A}$ with eigenvalues $1 \pm \epsilon$ would have yielded the same result.

Solutions to previous control questions (cont'd)

4.2 Eigenvalues follow from characteristic equation,

$$\det\left(\begin{array}{cc} H_{11}-\lambda & H_{12} \\ H_{12} & H_{22}-\lambda \end{array}\right) = 0$$

$$\longrightarrow \quad \lambda_{1,2} = \frac{H_{11}+H_{22}}{2} \pm \frac{H_{11}-H_{22}}{2}\sqrt{1+\frac{4H_{12}^2}{(H_{11}-H_{22})^2}}\,.$$

The eigenvectors are given by solutions of

$$\left(\begin{array}{cc} H_{11} & H_{12} \\ H_{12} & H_{22} \end{array}\right)\left(\begin{array}{c} \lambda_{i1} \\ \lambda_{i2} \end{array}\right) = \lambda_i \left(\begin{array}{c} \lambda_{i1} \\ \lambda_{i2} \end{array}\right)$$

$$\longrightarrow \quad \lambda_{i2} = \frac{\lambda_i - H_{11}}{H_{12}}\,\lambda_{i1} \longrightarrow \vec{\lambda}_i = \left(\begin{array}{c} H_{12} \\ \lambda_i - H_{11} \end{array}\right)\,.$$

Postulates for measurements in Quantum Mechanics

Postulate 3: All viable quantum mechanical observables can be represented as Hermitean operators.

Postulate 4: The only result of *one precise measurement* of an observable $\mathcal{A}$ is *one of the eigenvalues* of the associated Hermitean operator $\hat{A}$. The measurement will force the state vector of the system to becomes one the corresponding eigenvector.

Postulate 5: The result of *a series of measurements* of this observable over an ensemble of systems in the same state $|\Phi\rangle$, the *expectation value*, is given by

$$\langle\mathcal{A}\rangle_{|\Phi\rangle} = \frac{\left\langle\Phi\left|\hat{A}\right|\Phi\right\rangle}{\langle\Phi|\Phi\rangle}\,.$$

Expansion in eigenkets/eigenfunctions

- In postulate 3, *all observables* in Quantum Mechanics were connected with Hermitean operators, which have an orthonormal set of eigenvectors, spanning the full vector space as a base.
- This implies

> **Postulate 6:** Every ket representing a state of a dynamical system can be expressed as a *linear combination* of the normalised eigenkets of a Hermitean operator $\hat{O}$ associated to an observable $\mathcal{O}$.

Expansion in eigenkets/eigenfunctions and measurements

- Using postulate 6 and writing

$$|\psi\rangle = \sum_i c_i\,|\lambda_i\rangle \quad \text{with} \quad c_i = \langle\lambda_i|\psi\rangle \quad \text{and} \quad \sum_i |c_i|^2 = 1$$

therefore yields (with postulate 4)

$$\begin{aligned}\langle\mathcal{O}\rangle_\psi \equiv \left\langle\psi\left|\hat{O}\right|\psi\right\rangle &= \sum_{i,k} c_i^*\,c_k\,\left\langle\lambda_i\left|\hat{O}\right|\lambda_k\right\rangle \\ &= \sum_{i,k} c_i^*\,c_k\,\lambda_k\,\langle\lambda_i|\lambda_k\rangle = \sum_{i,k} c_i^*\,c_k\,\lambda_k\,\delta_{ik} = \sum_i |c_i|^2\,\lambda_i\,,\end{aligned}$$

which can be interpreted as an *weighted* average – the expectation value – of the eigenvalues of $\hat{O}$, with weights given by the probabilities $\mathcal{P}_i^{|\psi\rangle} = |c_i|^2$ of the system to be in the ith eigenstate, described by $|\psi\rangle$.

Expansion in eigenkets/eigenfunctions and measurements

- The terms $c_i = \langle\lambda_i|\psi\rangle$ are the *probability amplitudes* for the system to be found in $|\lambda_i\rangle$.
- As a by-product of postulate 4, a *single* measurement of $\mathcal{O}$ will lead to a collapse of the linear combination of $|\psi\rangle$ to a single eigenket $|\lambda_i\rangle$, which is chosen according to the probabilities $|c_i|^2$:

$$|\psi\rangle = \sum_i \langle\lambda_i|\psi\rangle\,|\lambda_i\rangle \xrightarrow{\mathcal{O}} |\lambda_i\rangle$$

- A subsequent immediate measurement of the same observable, $\mathcal{O}$, of the system then yields λ_i with certainty. This can be used to *prepare* a set of systems.

Partially continuous spectrum

- Now, assume a spectrum of $\hat{O}$, that consists of some discrete eigenvalues plus a range of continuous ones. Then:

$$|\psi\rangle = \sum_i c_i\,|\lambda_i\rangle + \int \mathrm{d}l\; c(l)\,|\lambda(l)\rangle\;,$$

with $c_i = \langle\lambda_i|\psi\rangle$ and, in a straightforward extension, $c(l) = \langle\lambda(l)|\psi\rangle$.

- Using the orthonormality of the eigenvectors

$$\langle\lambda_i|\lambda_j\rangle = \delta_{ij}\;,\quad \langle\lambda_i|\lambda(l)\rangle = 0\,,\quad \text{and}\quad \langle\lambda(k)|\lambda(l)\rangle = \delta(k-l)$$

therefore yields the expectation value for the observable $\mathcal{O}$

$$\langle\mathcal{O}\rangle_\psi = \sum_i |c_i|^2\,\lambda_i + \int \mathrm{d}l\,|c(l)|^2\,\lambda(l)\,.$$

Partially continuous spectrum - density of states

- As before, for the discrete part of the spectrum, $c_i = \langle\lambda_i|\psi\rangle$ denotes the *probability amplitude* for finding the system in state $|\lambda_i\rangle$, and therefore $|c_i|^2$ is the corresponding probability.
- For the continuous part, the states $\lambda(l)$ are lying dense, and one may introduce a *density of states*

$$\rho(l) = \frac{\mathrm{d}i}{\mathrm{d}l}\,,$$

  the number of states in a unit interval of l.
- This density can be used to normalise the eigenkets $|\lambda(l)\rangle$.

Operator functions

- Defining monomials of an operator $\hat{L}$ as $\hat{L}^n = \underbrace{\hat{L}\hat{L}\cdot\dots\cdot\hat{L}}_{n\,\text{factors}}$ allows to define operator functions $\mathcal{F}(\hat{L})$ through their Taylor-expansion

$$\mathcal{F}(\hat{L}) = f_0\hat{\mathbf{1}} + f_1\hat{L}^1 + f_2\hat{L}^2 + \dots$$

and in particular

$$e^{\hat{L}} = \exp(\hat{L}) = \sum_{n=0}^{\infty} \frac{1}{n!}\hat{L}^n.$$

- Differentiation of such functions with respect to operators is a bit cumbersome to define, but straightforward to exercise:

$$\frac{\partial}{\partial\hat{L}}(\mathcal{F}+\mathcal{G}) = \frac{\partial\mathcal{F}}{\partial\hat{L}} + \frac{\partial\mathcal{G}}{\partial\hat{L}}\,, \quad \frac{\partial}{\partial\hat{L}}(\mathcal{F}\mathcal{G}) = \frac{\partial\mathcal{F}}{\partial\hat{L}}\mathcal{G} + \mathcal{G}\frac{\partial\mathcal{G}}{\partial\hat{L}}\,,$$

$$\frac{\partial\hat{L}^n}{\partial\hat{L}} = n\hat{L}^{n-1}\,, \quad \frac{\partial e^{\hat{L}}}{\partial\hat{L}} = e^{\hat{L}}\,.$$

Commutators

The difference $\hat{L}\hat{M} - \hat{M}\hat{L} \equiv \left[\hat{L},\, \hat{M}\right] \equiv \left[\hat{L},\, \hat{M}\right]_-$ is called the commutator of the two operators and it has the following properties:

- $\left[\hat{L},\, \hat{M}\right] = -\left[\hat{M},\, \hat{L}\right]$ and, as a consequence, $\left[\hat{L},\, \hat{L}\right] = 0$;
- $\left[\hat{L},\, c\hat{\mathbf{1}}\right] = 0\ \forall c \in \mathbf{C}$;
- $\left[\hat{L},\, c\hat{M}\right] = c\left[\hat{L},\, \hat{M}\right]$;
- $\left[\hat{L}_1 + \hat{L}_2,\, \hat{M}\right] = \left[\hat{L_1},\, \hat{M}\right] + \left[\hat{L_2},\, \hat{M}\right]$;
- $\left[\hat{L}_1\hat{L}_2,\, \hat{M}\right] = \left[\hat{L_1},\, \hat{M}\right]\hat{L}_2 + \hat{L}_1\left[\hat{L_2},\, \hat{M}\right]$;
- $\left[\hat{M},\, \hat{L}_1\hat{L}_2\right] = \left[\hat{M},\, \hat{L_1}\right]\hat{L}_2 + \hat{L}_1\left[\hat{M},\, \hat{L_2}\right]$;
- $\left[\hat{L}_1,\, \left[\hat{L_2},\, \hat{L_3}\right]\right] + \left[\hat{L}_2,\, \left[\hat{L_3},\, \hat{L_1}\right]\right] + \left[\hat{L}_3,\, \left[\hat{L_1},\, \hat{L_2}\right]\right] = 0.$

Learning outcomes

- Results of measurements in Quantum Mechanics:
  Eigenvalue vs. expectation value.
- Operator functions
- Commutatorsand their basic properties

Control questions

5.1 The Hamilton operator $\hat{H}$ of a system and an operator $\hat{O}$ related to a measured quantity are given by

$$\hat{H} = \hbar\omega \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix} \quad \text{and} \quad \hat{O} = \mu \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} .$$

The system is described by a *normalised* state vector

$$|\psi\rangle = \sum_{i=1}^{2} c_i \, |v_i\rangle \ , \quad \text{where} \quad |v_1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad |v_2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} .$$

(a) What is the relation of the (potentially complex) quantities c_1 and c_2 to maintain $\langle\psi|\psi\rangle = 1$?

(b) What are possible energies that can be found when measuring the energy related to the state $|\psi\rangle$?

(c) What are the expectation values of $\hat{H}$ and $\hat{O}$, if the system is in a state $|\psi\rangle$?

Control questions

5.2 The Pauli matrices $\hat{\sigma}_{x,y,z}$ are given by

$$\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Prove by direct calculation that

$$[\hat{\sigma}_i, \hat{\sigma}_j] = 2i\epsilon_{ijk}\hat{\sigma}_k \quad \text{for} \quad \{i, j, k\} = \{1, 2, 3, \} = \{x, y, z\},$$

where ϵ_{ijk} is the Levi-Civita tensor (totally anti-symmetric tensor of rank 3) with $\epsilon_{123} = 1$.