Theoretical Physics II B – Quantum Mechanics

Lecture 4

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Solutions to previous control questions

3.1(a) Unitarity of $a\hat{U}$: $\hat{\mathbf{1}} \equiv (a\hat{U})^\dagger a\hat{U} = \hat{U}^\dagger \hat{U} a^* a$ is realised if $\hat{U}^\dagger \hat{U} \equiv \hat{\mathbf{1}}$, i.e. $\hat{U}$ unitary and $a^* a = 1$.

3.1(b) Unitarity of $\hat{U}\hat{V}$: $\hat{\mathbf{1}} \equiv (\hat{U}\hat{V})^\dagger \hat{U}\hat{V} = \hat{V}^\dagger \hat{U}^\dagger \hat{U}\hat{V} = \hat{V}^\dagger \hat{V}$, if $\hat{U}$ unitary, and the result equals the unit operator, if $\hat{U}$ unitary.

3.1(c) This is done by explicit calculation:

$$\hat{\mathbf{1}} \equiv \hat{V}^\dagger \hat{V} = \frac{1}{|\alpha|^2 + |\beta|^2} \begin{pmatrix} \alpha^* & -\beta \\ \beta^* & \alpha \end{pmatrix} \begin{pmatrix} \alpha & \beta \\ -\beta^* & \alpha^* \end{pmatrix}$$
$$= \frac{1}{|\alpha|^2 + |\beta|^2} \begin{pmatrix} \alpha\alpha^* + \beta\beta^* & 0 \\ 0 & \alpha\alpha^* + \beta\beta^* \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

as demanded.

Solutions to previous control questions

3.2(a) The unit operator looks like

$$\hat{\mathbf{1}} = \begin{pmatrix} 1 & 0 & \dots & 0 \\ 0 & 1 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 1 \end{pmatrix} \longrightarrow (\hat{\mathbf{1}})_{ik} = \delta_{ik} \quad \text{and} \quad \mathrm{Tr}\hat{\mathbf{1}} = \sum_{i=1}^{N} \delta_{ii} = N\,.$$

in N dimensions.

3.2(b) Remember matrix multiplication as "row $\times$ columns":

$$\hat{K} = \hat{L}\hat{M} \quad \longleftrightarrow \quad K_{ij} = \sum_{k=1} L_{ik}M_{kj} \equiv L_{ik}M_{kj}$$

using Einstein's convention of summing over repeated indices.

$$\mathrm{Tr}(\hat{L}\hat{M}) \equiv \sum_i (\hat{L}\hat{M})_{ii} = \sum_i \left(\sum_k L_{ik}M_{ki}\right) = \sum_k \left(\sum_i M_{ki}L_{ik}\right) = \mathrm{Tr}(\hat{M}\hat{L})$$

as requested.

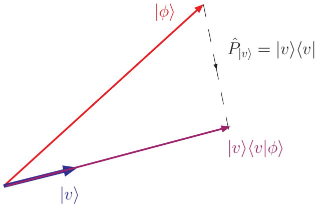
Special operators: Projection operators

Finally another class of operators is introduced, namely the projection operators $\hat{P}_{|v\rangle}$. For an arbitrary vector $|v\rangle$ with unit length $\langle v|v\rangle = 1$, they are defined through the

dyadic product: $\hat{P}_{|v\rangle} = |v\rangle\,\langle v|$.

- Projection operators are linear and Hermitean;
- they are **idempotent**: $\hat{P}^2_{|v\rangle} = \hat{P}_{|v\rangle}$;
- $\hat{P}_{|v\rangle}\hat{P}_{|u\rangle} = \hat{P}_{|u\rangle}\hat{P}_{|v\rangle} = 0$

  $\forall\,\langle u|v\rangle = 0$ (orthogonal kets);
- matrix elements: $\hat{P}_{|v\rangle;k'k} = \langle v'_k|v\rangle\,\langle v|v_k\rangle$.
- $\mathrm{Tr}\left(\hat{P_{|v\rangle}}\right) = 1$.



Eigenvalues and eigenvectors

Definition of eigenvalues λ_i and eigenvectors $|\lambda_i\rangle$ of an operator $\hat{O}$:

$$\boxed{\hat{O}\,|\lambda\rangle_i = \lambda_i\,|\lambda_i\rangle.}$$

Some nomenclature:

- The set of all eigenvalues $\{\lambda_i\}$ of an operator is called its *spectrum*;
- an eigenvalue is called *degenerate*, if it corresponds to more than one eigenvector.

Example: projection operators

The eigenvalue equation for a projection operator $\hat{P}_{|v\rangle}$ reads:

$$\hat{P}_{|v\rangle}\,|\lambda\rangle = |v\rangle\,\langle v|\lambda\rangle = \lambda\,|\lambda\rangle\;.$$

From this it can be read off that one eigenvalue is 1 with the corresponding eigenvector being $|v\rangle$. In addition, all other eigenvectors are orthogonal with respect to $|v\rangle$, with eigenvalue 0 - this is the only other way to guarantee that the right equal sign in the equation above holds true.
Therefore, these other eigenvectors, collectively denoted by $\{|v_{i,\perp}\rangle\}$ span an $(N-1)$-dimensional subspace of the original N-dimensional Hilbert space the kets live in.

Eigenproblem of Hermitean operators

Hermitean operators play a special role in Quantum mechanics, because

$$\boxed{\text{The eigenvalues of Hermitean operators are real, and their eigenvectors are orthogonal.}}$$

In fact, strictly speaking, this is true only for operators with non-degenerate spectra.

To see this, consider the eigenvalue equation $\hat{O}\,|\lambda\rangle_i = \lambda_i\,|\lambda_i\rangle$ and multiply from the left with another eigenvector $|\lambda_j\rangle$:

$$\left\langle \lambda_j \middle| \hat{O} \middle| \lambda_i \right\rangle = \lambda_i \langle \lambda_j | \lambda_i \rangle = \lambda_j^* \langle \lambda_j | \lambda_i \rangle \ ,$$

where the last part comes from applying the eigenvalue equation to $\langle \lambda_j|$. Then subtracting the two results yields

$$(\lambda_i - \lambda_j^*)\,\langle \lambda_i | \lambda_j \rangle = 0$$

and the reality of the eigenvalues becomes apparent for $i = j$, whereas the orthogonality of the eigenvectors can be seen by setting $i \neq j$.

Spectrum of an operator

- In lecture 3, it has been shown that the eigenvectors of an Hermitean operator $\hat{O}$ are orthogonal, with real eigenvalues, if the spectrum of $\hat{O}$ is non-degenerate.
- For degenerate spectra, *Schmidt's orthogonalisation procedure* allows to rearrange the eigenvectors corresponding to a degenerate eigenvalue into a mutually orthogonal set.
- In both cases, the eigenvectors can be normalised,
$$|\lambda_i\rangle \longrightarrow \frac{1}{\sqrt{\langle\lambda_i|\lambda_i\rangle}}\,|\lambda_i\rangle,$$
yielding an orthonormal base.

Reminder: orthonormal bases

- In previous lectures, orthonormal bases have been defined such that

$$\langle k|l\rangle = \begin{cases} \delta_{kl} & \text{if } k,\ l \text{ discrete} \\ \delta(k-l) & \text{if } k,\ l \text{ continuous.} \end{cases}$$

- They allow to expand all state vectors in them, yielding a *representation* of the ket with respect to a particular base:

$$|\phi\rangle = \begin{cases} \sum\limits_k |k\rangle\,\langle k|\phi\rangle & = \sum\limits_k |k\rangle\,\phi_k & \text{if } k \text{ discrete} \\ \int \mathrm{d}k\,|k\rangle\,\langle k|\phi\rangle & = \int \mathrm{d}k\,|k\rangle\,\phi(k) & \text{if } k \text{ continuous.} \end{cases}$$

  and giving rise to discrete components ϕ_k of the associated vector or to a wave function $\phi(k)$.

- This latter identification of $\phi(k)$ extents the original idea of a wave function, which typically has been applied to k indicating position or momentum space only.

Projection operators and closure

- Using such an orthonormal base, one can define *projection operators*

$$\hat{P}_k = |k\rangle\langle k| = \hat{P}(k)\,,$$

which are linear, Hermitean operators.

- Such projection operators are *idempotent*

$$\begin{aligned}\hat{P}_k\hat{P}_k &= |k\rangle\langle k|\cdot|k\rangle\langle k| = |k\rangle\langle k| = \hat{P}_k\\ \hat{P}_k\hat{P}_l &= |k\rangle\langle k|\cdot|l\rangle\langle l| = 0\,.\end{aligned}$$

- They exhibit closure (i.e. add up to 1):

$$1 = \begin{cases}\sum\limits_k \hat{P}_k & \text{for} \quad k \text{ discrete}\\ \int \mathrm{d}k\hat{P}(k) & \text{for} \quad k \text{ continuous.}\end{cases}$$

Unitary operators, once more

- Remember unitary operators $\hat{U}$ which by definition satisfy

$$\hat{U}^\dagger = \hat{U}^{-1}\,.$$

- Unitary transformations of kets leaves their scalar products invariant:

$$\left\langle \hat{U}\phi|\hat{U}\chi\right\rangle = \langle\phi|\,\hat{U}^\dagger\hat{U}\,|\chi\rangle = \langle\phi|\chi\rangle\;.$$

- Also "operator sandwiches" remain invariant:

$$\left\langle \phi\left|\hat{A}\right|\chi\right\rangle = \langle\phi|\,\hat{U}^\dagger\hat{U}\hat{A}\hat{U}^\dagger\hat{U}\,|\chi\rangle = \langle\hat{U}\phi|\hat{A}'|\hat{U}\chi\rangle = \left\langle \phi'\left|\hat{A}'\right|\chi'\right\rangle\;.$$

- Under unitary transformations, operators remain Hermitean:

$$\hat{A}' = \hat{U}\hat{A}\hat{U}^\dagger \;\longleftrightarrow\; \hat{A}'^\dagger = (\hat{U}\hat{A}\hat{U}^\dagger)^\dagger = \hat{U}\hat{A}^\dagger\hat{U}^\dagger\,.$$

Unitary operators, once more

- Eigenvalues of transformed matrices equal the original ones:

$$\begin{aligned}\hat{A}\,|\lambda\rangle = \hat{A}\hat{U}^\dagger\hat{U}\,|\lambda\rangle &= \lambda\hat{U}^\dagger\hat{U}\,|\lambda\rangle\\ \hat{U}\hat{A}\hat{U}^\dagger\hat{U}\,|\lambda\rangle &= \hat{U}\lambda\hat{U}^\dagger\hat{U}\,|\lambda\rangle\\ \hat{A}'\,|\lambda'\rangle &= \lambda\,|\lambda'\rangle\,.\end{aligned}$$

- Traces are invariant under unitary transformations

$$\begin{aligned}\mathrm{Tr}\hat{A}' &= \sum_m(\hat{A}')_{mm} = \sum_{m,k,l}(\hat{U})_{mk}(\hat{A})_{kl}(\hat{U}^\dagger)_{lm}\\ &= \sum_{k,l}\left[\sum_m(\hat{U}^\dagger)_{lm}(\hat{U})_{mk}\right](\hat{A})_{kl} = \sum_{k,l}\delta_{kl}(\hat{A})_{kl}\\ &= \sum_k(\hat{A})_{kk} = \mathrm{Tr}\hat{A}\,.\end{aligned}$$

Unitary base transformations

- Consider the action of an unitary transformation on the *representation* of kets through their components.
- Such a transformation may be seen in two ways:
  1. Active: The operators act on kets, "moving" them around,

     $$|\phi\rangle \xrightarrow{V} |\phi'\rangle = \hat{V}\,|\phi\rangle \;\;, \quad |v_k\rangle = \mathrm{const.}\,,$$

     but keeping the base vectors fixed;
  2. Passive: The base vectors are "moved in the opposite direction",

     $$|v_k\rangle \xrightarrow{U} |v_k'\rangle = \hat{U}\,|v_k\rangle \;\;, \quad |\phi\rangle = \mathrm{const.}\,,$$

     where $\hat{V} = \hat{U}^\dagger$ and the physical kets stay fixed.
     This is the case when discussing a *base transformation*.

Unitary base transformations

- Assume you want to go from an orthonormal set of old base vectors $\{|v_k\rangle\}$ to another set of new base vectors $\{|u_l\rangle\}$, through a transformation T: $\{|v_k\rangle\} \xrightarrow{T} \{|u_l\rangle\}$

  Of course, being bases, both sets have an identical number of members. This means that, of course, the dimension of the space spanned by them remains fixed.

- Express the new base vectors through the old ones - i.e. re-expand the new base in terms of the old one:
$$|u_l\rangle = \sum_k |v_k\rangle \langle v_k|u_l\rangle.$$
  Remark: As before, the object $|v_k\rangle\langle v_k|$ has matrix form (a so-called dyadic product), and is known as *projection operator*.

  Cf. slides 14 and 16 of lecture 3 for a quick recap.

- The transformation operator (matrix) $\hat{T}$ is given by
$$\hat{T}_{kl} = \langle v_k|u_l\rangle,$$
  its components are the components of the new base vectors with respect to the old ones.

Unitary base transformations (cont'd)

- Demanding that the new base vectors are orthonormal translates into

$$\delta_{kl} \equiv \langle u_k | u_l \rangle = \sum_{i,j} \Big(\langle u_k | v_i \rangle \langle v_i | \cdot | v_j \rangle \langle v_j | u_l \rangle \Big)$$
$$= \sum_{i,j} \langle u_k | v_i \rangle \langle v_i | v_j \rangle \langle v_j | u_l \rangle = \sum_i \langle u_k | v_i \rangle \langle v_i | u_l \rangle = \sum_i (\hat{T})^*_{ki} (\hat{T})_{il}$$

  or, in operator notation, $\hat{\mathbf{1}} = \hat{T}^\dagger \hat{T}$

- In other words, the transformation operator transforming one orthonormal base into another one is *unitary*.

Back-transformation

- Of course, conversely, the old base vectors $\{|v_k\rangle\}$ can be expressed through the new ones:
$$|v_k\rangle = \sum_l |u_l\rangle \langle u_l|v_k\rangle \,.$$
- This implies that the matrix elements of the back-transformation $\{|u_l\rangle\} \xrightarrow{S} \{|v_k\rangle\}$ are given by
$$(\hat{S})_{lk} = \langle u_l|v_k\rangle = (\langle v_k|u_l\rangle)^* = (\hat{T})^*_{kl} = (\hat{T}^\dagger)_{lk}.$$
- Therefore, in the new coordinates, an operator $\hat{A}$ reads
$$\hat{A}\Big|_u = \hat{T}^\dagger\ \hat{A}\Big|_v\ \hat{T}\,,$$
where the operator in the old base $\{|v_k\rangle\}$ is given by $\hat{A}\Big|_v$.

Continuous base vectors

- The above properties also apply for transformations involving continuous base vectors. The new base vectors $|u(l)\rangle$ emerging from the old ones $|v(k)\rangle$ through the transformation $|v(k)\rangle \xrightarrow{T} |u(l)\rangle$ can be expressed in terms of these old base as
$$|u(l)\rangle = \int \mathrm{d}k\, |v(k)\rangle\, \langle v(k)|u(l)\rangle,$$
and the components of the transformation operator $\hat{T}$, as before are given by the *continuous* elements $\hat{T}(k,\, l) = \langle v(k)|u(l)\rangle$.
- Demanding an orthonormal bases implies $\langle u(k)|u(l)\rangle = \delta(k-l)$:
$$\begin{aligned}\delta(k-l) \equiv \langle u(k)|u(l)\rangle &= \int \mathrm{d}i\mathrm{d}j\, \left(\langle u(k)|v(i)\rangle\, \langle v(i)|v(j)\rangle\, \langle v(j)|u(l)\rangle\right)\\ &= \int \mathrm{d}i\, \left(\langle u(k)|v(i)\rangle\, \langle v(i)|u(l)\rangle\right) = \int \mathrm{d}i\, \hat{T}^*(k,i)\hat{T}(i,\, l)\,,\end{aligned}$$
the integral form of the operator equation $\hat{\mathbf{1}} = \hat{T}^\dagger\hat{T}$.

Continuous base vectors: An example

- Consider the transformation from a base given by "position"-kets $|x\rangle$ in one dimension to one given by "momentum"-kets $|p\rangle$:

  For the moment, let's forget about some tricky factors of $\hbar$. $|x\rangle \xrightarrow{T} |p\rangle$, where both bases are orthonormal:

$$\langle x|x'\rangle = \delta(x-x') \text{ and } \langle p|p'\rangle = \delta(p-p').$$

- A state ket $|\phi\rangle$ in both bases is given by

$$|\phi\rangle = \int\limits_{-\infty}^{\infty} \mathrm{d}x\,|x\rangle\;\phi(x) = \int\limits_{-\infty}^{\infty} \mathrm{d}p\,|p\rangle\;\tilde{\phi}(p),$$

$$\phi(x) = \frac{1}{\sqrt{2\pi}}\int\limits_{-\infty}^{\infty} \mathrm{d}p\,e^{ipx}\tilde{\phi}(p) \text{ and } \tilde{\phi}(p) = \frac{1}{\sqrt{2\pi}}\int\limits_{-\infty}^{\infty} \mathrm{d}x\,e^{-ipx}\phi(x).$$

Continuous base vectors: An example (cont'd)

- The transformation matrix is given by

$$\langle x|p\rangle = \hat{T}(x,\, p) = \frac{1}{\sqrt{2\pi}}\, e^{ipx},$$

and because, as we know, all functions can be Fourier-transformed, we know that we go from one *complete* base to another.

- Using this to evaluate the scalar products of the base vectors yields

$$\langle x'|x\rangle = \frac{1}{2\pi}\int\limits_{-\infty}^{\infty} \mathrm{d}p\, \langle x'|p\rangle\, \langle p|x\rangle = \frac{1}{2\pi}\int\limits_{-\infty}^{\infty} \mathrm{d}p\, e^{ip(x'-x)} = \delta(x-x')$$

and similarly $\langle p'|p\rangle = \delta(p-p')$.

Learning outcomes

- Eigenvalues and eigenvectors.
- Unitary transformations for transformations from one orthonormal base to another.
- Using eigenkets of an Hermitean operator as orthonormal base.

Control questions

4.1 Consider a two-dimensional system where the kets $|\psi_1\rangle$ and $|\psi_2\rangle$ form an orthonormal basis. In this basis the operator $\hat{A}$ is given by

$$\hat{A}\Big|_\psi = \left(\begin{array}{cc} \left\langle\psi_1\left|\hat{A}\right|\psi_1\right\rangle & \left\langle\psi_1\left|\hat{A}\right|\psi_2\right\rangle \\ \left\langle\psi_2\left|\hat{A}\right|\psi_1\right\rangle & \left\langle\psi_2\left|\hat{A}\right|\psi_2\right\rangle \end{array}\right) = \left(\begin{array}{cc} 1 & \epsilon \\ \epsilon & 1 \end{array}\right).$$

What is the representation of this operator in a basis given by

$$|\phi_{1,2}\rangle = \frac{1}{\sqrt{2}}\left(|\psi_1\rangle \pm |\psi_2\rangle\right)?$$

Control questions

4.2 What are the eigenkets and eigenvalues of the Hamiltonian given by

$$\hat{H} = H_{11}|1\rangle\langle 1| + H_{12}|1\rangle\langle 2| + H_{21}|2\rangle\langle 1| + H_{22}|2\rangle\langle 2|\,,$$

where all entries $H_{ij} \in \mathbf{R}$ are real numbers and where, in particular, $H_{12} = H_{21}$.