Prof. Dr. Viatcheslav Mukhanov Winter term 2019/2020

Exercises on Quantum Mechanics II (TM1/TV)

Solution 2, discussed October 28 - November 1, 2019

Exercise 9 (central tutorial)

(i) Show that if $\hat{A}\hat{B} = \mathbb{1} = \hat{C}\hat{A}$ then we have

$$\hat{B} = \hat{A}^{-1} = \hat{C}.$$

Remember that the inverse operator $\hat{A}^{-1}$ satisfies $|\psi\rangle = \hat{A}\,|\chi\rangle$ if and only if $|\chi\rangle = \hat{A}^{-1}\,|\psi\rangle$.

(ii) Given an example of operators $\hat{A}$ and $\hat{B}$ in Hilbert space for which $\hat{A}\hat{B} = \mathbb{1}$ holds but for which $\hat{B}\hat{A} \neq \mathbb{1}$.

(iii) Let $\hat{A}$ be an operator such that $\hat{A}^2 = \lambda\mathbb{1}$ where $\lambda \neq 1$ is a complex number. Write $\left(\hat{A} + \mathbb{1}\right)^{-1}$ explicitly in terms of $\hat{A}$.

Solution

(i) To prove that $\hat{B} = \hat{C}$ we can multiply the first equation by $\hat{C}$ from the left:

$$\hat{C} \overset{(1)}{=} \hat{C}(\hat{A}\hat{B}) = (\hat{C}\hat{A})\hat{B} \overset{(2)}{=} \hat{B}.$$

To show that $\hat{B} = \hat{C}$ is the inverse operator to $\hat{A}$, we first assume that $|\psi\rangle = \hat{A}\,|\chi\rangle$ and act on this with $\hat{C}$ and find $|\chi\rangle = \hat{C}\,|\psi\rangle$ which shows one direction of the equivalence. The other direction can be shown analogously by acting with $\hat{B}$.

(ii) We can consider a rescaled version of ladder operator in the harmonic oscillator. Remember that there we have an orthonormal basis of states $|n\rangle$ where $n = 0, 1, 2, \ldots$ and creation and annihilation operator which act as

$$\hat{a}^\dagger\,|n\rangle = \sqrt{n+1}\,|n+1\rangle\,, \qquad \hat{a}\,|n\rangle = \sqrt{n}\,|n-1\rangle\,.$$

Consider now modified ladder operators such that

$$\hat{b}^\dagger\,|n\rangle = |n+1\rangle$$

and

$$\hat{b}\,|n\rangle = \begin{cases} |n-1\rangle\,, & n > 0 \\ 0, & n = 0 \end{cases}$$

We can now choose $\hat{A} = \hat{b}$ and $\hat{B} = \hat{b}^\dagger$. Acting on any basis state we find

$$\hat{A}\hat{B}\,|n\rangle = \hat{b}\hat{b}^\dagger\,|n\rangle = \hat{b}\,|n+1\rangle = |n\rangle$$

so $\hat{A}\hat{B} = \mathbb{1}$ but acting on the ground state $|0\rangle$ we have

$$\hat{B}\hat{A}\,|0\rangle = \hat{b}^\dagger\hat{b}\,|0\rangle = 0$$

so $\hat{A}$ and $\hat{B}$ are not inverse of each other.

(iii) Since $\hat{A}$ squares to something proportional to identity, any function of $\hat{A}$ that can be written as power series in $\hat{A}$ can be reduced to the form

$$\alpha\hat{\mathbb{1}} + \beta\hat{A}.$$

Let's try this ansatz for an inverse of $\hat{A}$:

$$\hat{\mathbb{1}} = \left(\hat{A}+\hat{\mathbb{1}}\right)\left(\hat{A}+\hat{\mathbb{1}}\right)^{-1} = \left(\hat{A}+\hat{\mathbb{1}}\right)\left(\alpha\hat{\mathbb{1}}+\beta\hat{A}\right) = \alpha\hat{\mathbb{1}}+\alpha\hat{A}+\beta\hat{A}+\beta\hat{A}^2$$

The left and right hand side are equal if α and β satisfy

$$\alpha+\beta = 0, \qquad 1 = \alpha+\beta\lambda.$$

These equations have unique solution

$$\alpha = \frac{1}{1-\lambda}, \qquad \beta = -\frac{1}{1-\lambda}$$

which gives us a candidate for an inverse operator

$$\left(\hat{A}+\hat{\mathbb{1}}\right)^{-1} = \frac{\hat{\mathbb{1}}-\hat{A}}{1-\lambda}.$$

One can now easily check that this operator is not only right inverse (which is true by our construction) but also a left inverse.

Alternative solution: we can also use the geometric series to find the inverse operator. We have

$$\left(\hat{A}+\hat{\mathbb{1}}\right)^{-1} = \sum_{k=0}^{\infty}\left(-\hat{A}\right)^k = \sum_{l=0}^{\infty}\lambda^l + (-\hat{A})\sum_{m=0}^{\infty}\lambda^m = \frac{\hat{\mathbb{1}}-\hat{A}}{1-\lambda}$$

where in the middle part we split the sum over all integers to a sum over all even integers $2l$ plus a sum over all odd integers $2m+1$.

Exercise 10

Consider the operator $\hat{A} = \frac{d}{dx}$.

(i) Use the Taylor expansion to find out how $e^{\alpha\hat{A}}$ acts on wavefunctions. Interpret the result physically.

(ii) How do operators $\hat{B} \equiv \sinh(\alpha\hat{A})$ and $\hat{C} \equiv \sin(\alpha\hat{A})$ act on wavefunctions?

Solution

(i) Acting with $e^{\alpha\hat{A}}$ on a function $\psi(x)$ we have

$$e^{\alpha\hat{A}}\psi(x) = e^{\alpha\frac{d}{dx}}\psi(x) = \sum_{k=0}^{\infty}\frac{\alpha^k}{k!}\left(\frac{d}{dx}\right)^k\psi(x) = \psi(x+\alpha)$$

so the resulting operator corresponds to a space translation of the wavefunction.

(ii) We have

$$\hat{B} = \sinh\left(\alpha\hat{A}\right) = \frac{e^{\alpha\hat{A}} - e^{-\alpha\hat{A}}}{2}.$$

By the result of the previous exercise this acts on $\psi(x)$ as

$$\hat{B}\psi(x) = \frac{1}{2}\left(\psi(x+\alpha) - \psi(x-\alpha)\right).$$

Replacing $\alpha \to i\alpha$ and dividing by i we find

$$\hat{C}\psi(x) = \frac{i}{2}\left(\psi(x-i\alpha) - \psi(x+i\alpha)\right).$$

Exercise 11

Find $\hat{A}^\dagger$ for $\hat{A} = |\varphi\rangle\langle\psi|$. Remember that $\hat{A}^\dagger$ is defined such that for any two vectors $|\psi\rangle$ and $|\chi\rangle$ we have $\left\langle\psi|\hat{A}\chi\right\rangle = \left\langle\hat{A}^\dagger\psi|\chi\right\rangle$.

Solution By definition of the conjugate operator we have

$$\langle\chi|\hat{A}^\dagger|\eta\rangle = \left(\hat{A}|\chi\rangle, |\eta\rangle\right) = \left(\langle\psi|\chi\rangle|\varphi\rangle, |\eta\rangle\right) = \langle\chi|\psi\rangle\langle\varphi|\eta\rangle$$

Comparing both sides we see that

$$\hat{A}^\dagger = |\psi\rangle\langle\varphi|.$$

Exercise 12

(i) Show that for an orthonormal basis $|\delta_j\rangle$ we have the completeness relation

$$\sum_k |\delta_k\rangle\langle\delta^k| = \hat{\mathbb{1}}.$$

(ii) Consider a product of two operators $\hat{C} = \hat{A}\hat{B}$. Remember that the matrix elements of the operator $\hat{A}$ in the orthonormal basis $|\delta_j\rangle$ were defined as $A^j{}_k \equiv \langle\delta^j|\hat{A}|\delta_k\rangle$. Show that the components of $\hat{C}$ are given by the usual product of matrices.

(iii) Show that the operator $\hat{A}$ can be reconstructed from its components via

$$\hat{A} = \sum_{jk} A^j{}_k |\delta_j\rangle\langle\delta^k|$$

Solution

(i) Since we have an orthonormal basis, any vector $|\psi\rangle$ can be expanded as

$$|\psi\rangle = \sum_j a_j|\delta_j\rangle$$

and

$$\langle\delta^k|\psi\rangle = \sum_j a_j\langle\delta^k|\delta_j\rangle = a_k.$$

Let us now apply $\sum_k |\delta^k\rangle\langle\delta_k|$ to an any vector $|\psi\rangle$

$$\sum_k |\delta_k\rangle\langle\delta^k|\psi\rangle = \sum_k a_k|\delta_k\rangle = |\psi\rangle.$$

Since this holds for all vectors, we see that $\sum_k |\delta^k\rangle\langle\delta_k| = \hat{\mathbb{1}}$.

(ii) We have

$$(\hat{C})^j{}_l = \langle\delta^j|\hat{A}\hat{B}|\delta_l\rangle = \sum_k \langle\delta^j|\hat{A}|\delta_k\rangle\langle\delta^k|\hat{B}|\delta_l\rangle = \sum_k A^j{}_k B^k{}_l$$

which is the usual rule for matrix multiplication. In the middle equation we inserted the completeness relation.

(iii) Plugging in the expression for components

$$\sum_{j,k}\langle\delta^j|\hat{A}|\delta_k\rangle|\delta_j\rangle\langle\delta^k| = \sum_{j,k}|\delta_j\rangle\langle\delta^j|\hat{A}|\delta_k\rangle\langle\delta^k| = \hat{A}.$$

Exercise 13

It was shown in the lecture that the matrix elements of the conjugate operator are

$$\langle\delta^j|\hat{C}^\dagger|\delta_l\rangle = \left[\langle\delta^l|\hat{C}|\delta_j\rangle\right]^*,$$

i.e. the matrix of components is complex conjugate transpose. Use this to show that $(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger\hat{A}^\dagger$.

Solution Let us calculate

$$\begin{aligned}\langle\delta^j|\left(\hat{A}\hat{B}\right)^\dagger|\delta_l\rangle &= \left[\langle\delta^l|\hat{A}\hat{B}|\delta_j\rangle\right]^* = \sum_k\left[\langle\delta^l|\hat{A}|\delta_k\rangle\langle\delta^k|\hat{B}|\delta_j\rangle\right]^* = \sum_k\left[\langle\delta^l|\hat{A}|\delta_k\rangle\right]^*\left[\langle\delta^k|\hat{B}|\delta_j\rangle\right]^* \\ &= \sum_k\left[\langle\delta^k|\hat{A}^\dagger|\delta_l\rangle\right]\left[\langle\delta^j|\hat{B}^\dagger|\delta_k\rangle\right] = \sum_k\langle\delta^j|\hat{B}^\dagger|\delta_k\rangle\langle\delta^k|\hat{A}^\dagger|\delta_l\rangle \\ &= \langle\delta^j|\hat{B}^\dagger\hat{A}^\dagger|\delta_l\rangle\,.\end{aligned}$$

Exercise 14 (central tutorial)

Consider a change of orthonormal basis $|\delta\rangle \to \left|\tilde{\delta}\right\rangle$ in the Hilbert space described by $U^j{}_k \equiv \left\langle\tilde{\delta}^j|\delta_k\right\rangle$.

(i) Show that $U^j{}_k$ are components of unitary matrix, i.e. $(U^\dagger)^j{}_k = (U^k{}_j)^* = (U^{-1})^j{}_k$.

(ii) Show that the components of bra vectors in the old and in the new basis are related by

$$\tilde{\psi}_k = \sum_j \psi_j (U^\dagger)^j{}_k$$

(iii) Show that the matrix elements of operators transform as

$$\tilde{A}^j_m = \sum_{kl} U^j{}_k A^k{}_l (U^\dagger)^l{}_m.$$

Solution

(i) We have

$$\left\langle\delta^j|\tilde{\delta}_k\right\rangle = \left\langle\tilde{\delta}^k|\delta_j\right\rangle^* = (U^k{}_j)^* = (U^\dagger)^j{}_k.$$

To see that this is an inverse of U, calculate

$$(UU^\dagger)^j{}_k = \sum_l U^j{}_l (U^\dagger)^l{}_k = \sum_l \left\langle\tilde{\delta}^j|\delta_l\right\rangle\left\langle\delta^l|\tilde{\delta}_k\right\rangle = \left\langle\tilde{\delta}^j|\tilde{\delta}_k\right\rangle = \delta^j_k = (\mathbb{1})^j_k.$$

Multiplication in opposite order is analogous.

(ii) Expressing the bra vector in two bases,

$$\sum_k \tilde{\psi}_k\left\langle\tilde{\delta}^k\right| = \langle\psi| = \sum_j \psi_j\langle\delta^j| = \sum_{j,k}\psi_j\left\langle\delta^j|\tilde{\delta}_k\right\rangle\left\langle\tilde{\delta}^k\right|$$

Comparing both sides we see that

$$\tilde{\psi}_k = \sum_j \psi_j\left\langle\delta^j|\tilde{\delta}_k\right\rangle = \sum_j \psi_j (U^\dagger)^j{}_k$$

(iii) The matrix elements of $\hat{A}$ in the new basis are

$$\tilde{A}^j_m = \left\langle\tilde{\delta}^j\right|\hat{A}\left|\tilde{\delta}_m\right\rangle = \sum_{k,l}\left\langle\tilde{\delta}^j|\delta_k\right\rangle\langle\delta^k|\hat{A}|\delta_l\rangle\left\langle\delta^l|\tilde{\delta}_m\right\rangle = \sum_{k,l} U^j{}_k A^k{}_l (U^\dagger)^l{}_m.$$

Exercise 15

Consider a Hermitian operator $\hat{A}$ and a unitary operator $\hat{U}$.

(i) Show that the trace of the operator $\hat{A}$ is independent of the choice of the basis. What property of the trace follows from the hermiticity of $\hat{A}$?

(ii) How are spectra of $\hat{A}$ and of $\hat{U}\hat{A}\hat{U}^\dagger$ related?

Solution

(i) Let us calculate the trace of $\hat{A}$ in the new basis

$$\sum_j \left\langle \tilde{\delta}^j \right| \hat{A} \left| \tilde{\delta}_j \right\rangle = \sum_{j,k,l} \left\langle \tilde{\delta}^j | \delta_k \right\rangle \langle \delta^k | \hat{A} | \delta_l \rangle \left\langle \delta^l | \tilde{\delta}_j \right\rangle = \sum_{k,l} \langle \delta^l | \delta_k \rangle \langle \delta^k | \hat{A} | \delta_l \rangle = \sum_k \langle \delta^k | \hat{A} | \delta_k \rangle .$$

In particular we can choose a basis which diagonalizes $\hat{A}$. In this basis the eigenvalues are real (because $\hat{A}$ is Hermitian) so also their sum, i.e. the trace is real.

(ii) Recall that $\lambda \in \mathbb{C}$ is in the spectrum of $\hat{A}$ if there exists a vector $|\psi\rangle$ such that

$$\hat{A} |\psi\rangle = \lambda |\psi\rangle .$$

Acting on this equation with $\hat{U}$ from the left, we find that the vector $|\eta\rangle \equiv \hat{U} |\psi\rangle$ satisfies the equation

$$\hat{U}\hat{A}\hat{U}^\dagger |\eta\rangle = \hat{U}\hat{A}\hat{U}^\dagger \hat{U} |\psi\rangle = \lambda \hat{U} |\psi\rangle = \lambda |\eta\rangle ,$$

i.e. is an eigenvector of $\hat{U}\hat{A}\hat{U}^\dagger$ with the same eigenvalue λ. Since $\hat{U}$ is unitary (and so in particular invertible), this provides a one-to-one correspondence between eigenvectors of $\hat{A}$ and $\hat{U}\hat{A}\hat{U}^\dagger$.

Exercise 16

Consider a linear operator acting on a Hilbert space such that it maps one orthonormal basis into another one, $\hat{U} |\delta_j\rangle = |\delta'_j\rangle$. How can you write this operator in terms of basis vectors? Find its hermitian conjugate.

Solution

(i) If we consider action of $\sum_k |\delta'_k\rangle \langle \delta^k|$ on basis vectors,

$$\sum_k |\delta'_k\rangle \langle \delta^k | \delta_j \rangle = |\delta'_j\rangle$$

which is exactly how $\hat{U}$ acts.

(ii) By the definition of conjugate operator, we have

$$\langle \delta^j | \hat{U}^\dagger = \langle \delta'^j |$$

which is the same as the action of $\sum_k |\delta_k\rangle \langle \delta'^k|$,

$$\langle \delta^j | \sum_k |\delta_k\rangle \langle \delta'^k | = \langle \delta'^j | .$$

Exercise 17 (central tutorial)

The position operator $\hat{x}$ is hermitian. The momenum operator satisfies the commutation relation

$$[\hat{x}, \hat{p}] = i\hbar \mathbb{1}.$$

Does this imply that $\hat{p}$ is a hermitian operator? Can there exist finite dimensional matrices $\hat{x}$ and $\hat{p}$ which satisfy these commutation relations?

Solution

(i) The commutation relations don't force $\hat{p}$ to be hermitian. If we had a hermitian solution (like the standard $\hat{p} = -i\hbar\frac{\partial}{\partial x}$) we can add to it any complex multiple of $\hat{x}$ without spoiling the commutation relations. Now we have

$$(\hat{p} + \alpha\hat{x})^\dagger = \hat{p}^\dagger + \alpha^* \hat{x}^\dagger = \hat{p} + \alpha^* \hat{x}$$

which agrees with $\hat{p} + \alpha\hat{x}$ only if α is real. So taking α with non-vanishing imaginary part is a counter-example to the question.

(ii) There cannot exist any finite-dimensional matrices $\hat{x}$ and $\hat{p}$ which would satisfy the canonical commutation relations. The reason for it is that the trace of any commutator vanishes by cyclicity of the trace,

$$\mathrm{Tr}\left[\hat{A},\hat{B}\right] = \mathrm{Tr}\left(\hat{A}\hat{B} - \hat{B}\hat{A}\right) = \mathrm{Tr}\left(\hat{A}\hat{B} - \hat{A}\hat{B}\right) = 0$$

while the trace of the identity matrix on the right-hand side is the dimension of the vector space. We thus find an equation

$$0 = \mathrm{Tr}\left[\hat{x},\hat{p}\right] = i\hbar\,\mathrm{Tr}\,\mathbb{1} = i\hbar n$$

which is a contradiction with finite dimensionality of the vector space.

Exercise 18 (central tutorial)

Check by direct calculation that

$$\int dq'' \left[X^{q}{}_{q''} P^{q''}{}_{q'} - P^{q}{}_{q''} X^{q''}{}_{q'} \right] = i\hbar \delta^{q}_{q'} = i\hbar\delta(q-q')$$

where the matrix elements of $\hat{X}$ are $X^{q}{}_{q'} \equiv \langle q|\,\hat{X}\,|q'\rangle$ and similarly for $\hat{P}$.

Solution We can rewrite the formula in bra-ket notation as

$$\int dq'' \left[\langle q|\,\hat{X}\,|q''\rangle \langle q''|\,\hat{P}\,|q'\rangle - \langle q|\,\hat{P}\,|q''\rangle \langle q''|\,\hat{X}\,|q'\rangle \right] = i\hbar \langle q|q'\rangle = i\hbar\delta(q-q')$$

Now we have the basic identification between vectors and wave functions

$$\psi(q) = \langle q|\psi\rangle$$

and so

$$\langle q|\,\hat{X}\,|\psi\rangle = q\psi(q), \qquad \langle q|\,\hat{P}\,|\psi\rangle = -i\hbar\partial_q\psi(q).$$

Choosing $|\psi\rangle = |q'\rangle$ so that $\psi(q) = \langle q|q'\rangle = \delta(q-q')$ we find the matrix elements

$$\langle q|\,\hat{X}\,|q'\rangle = q\delta(q-q'), \qquad \langle q|\,\hat{P}\,|q'\rangle = -i\hbar\partial_q\delta(q-q') = -i\hbar\delta'(q-q').$$

We can now use this in the equation above

$$\begin{aligned} I &= \int dq'' \left[\langle q|\,\hat{X}\,|q''\rangle \langle q''|\,\hat{P}\,|q'\rangle - \langle q|\,\hat{P}\,|q''\rangle \langle q''|\,\hat{X}\,|q'\rangle \right] \\ &= \int dq'' \left[q\delta(q-q'')(-i\hbar)\delta'(q''-q') - (-i\hbar)\delta'(q-q'')q''\delta(q''-q') \right] \\ &= q(-i\hbar)\delta'(q-q') - (-i\hbar)\delta'(q-q')q' = -i\hbar(q-q')\delta'(q-q') \\ &= i\hbar\delta(q-q'). \end{aligned}$$

We used the relation $x\delta'(x) = -\delta(x)$ which follows by acting on test function $\phi(x)$,

$$\int x\delta'(x)\phi(x)dx = -\int \delta(x)\frac{d}{dx}(x\phi(x))dx = -\int \delta(x)\left[\phi(x) + x\phi'(x)\right]dx = -\int \delta(x)\phi(x)dx$$