Advanced Quantum Mechanics

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Exercise sheet 1 **Due: Sunday April 9 at 24:00**

This sheet is a recap, so you might want to look up old lecture notes. You can also take a look at the appendices of the current lecture notes.

1 Operators, matrices and functions

In this exercise we take a look at the relation between operators and their matrix-representations. For the sake of extra clarity, we will in this exercise put a hat, $\hat{Q}$ on the operators, while denoting their matrix representations with bold letter $\boldsymbol{Q}$.[1] Recall that for an orthonormal basis $\{|a_k\rangle\}_k$ we have the orthonormality condition $\langle a_{k'}|a_k\rangle = \delta_{k,k'}$ and the resolution of identity $\sum_k |a_k\rangle\langle a_k| = \hat{1}$.

a) *Use the resolution of identity to show that an operator* $\hat{Q}$ *and its matrix representation* $\boldsymbol{Q}^{(a)}_{k',k} = \langle a_{k'}|\hat{Q}|a_k\rangle$ *in the basis* $\{|a_k\rangle\}_k$ *are related as*

$$\hat{Q} = \sum_{k',k} \boldsymbol{Q}^{(a)}_{k',k} |a_{k'}\rangle\langle a_k|.$$

(1 point)

b) Let $\{|b_l\rangle\}_l$ be an additional orthonormal basis. Let $\boldsymbol{Q}^{(b)}_{l',l} = \langle b_{l'}|\hat{Q}|b_l\rangle$ be the matrix representation in basis $\{|b_l\rangle\}_l$. *Express* $\boldsymbol{Q}^{(b)}_{l',l}$ *in terms of* $\boldsymbol{Q}^{(a)}_{k',k}$. **(2 points)**

c) Let $\boldsymbol{Q}$ be the matrix representation of $\hat{Q}$, i.e., $\boldsymbol{Q}$ has matrix elements $\boldsymbol{Q}_{k',k} = \langle a_{k'}|\hat{Q}|a_k\rangle$, where we have skipped the superscript (a). *Show that*

$$\hat{Q}^n = \sum_{k',k} |a_{k'}\rangle(\boldsymbol{Q}^n)_{k',k}\langle a_k|, \quad n = 1, 2, \ldots.$$

Hint: One can for example use a proof by induction. **(3 points)**

d) Given a function $f : \mathbb{R} \to \mathbb{R}$ (or $f : \mathbb{C} \to \mathbb{C}$) there are various methods to define the function $f(\hat{Q})$ of an operator $\hat{Q}$ (or the function $f(\boldsymbol{Q})$ of a (square) matrix $\boldsymbol{Q}$). If f possesses a (well-defined) Taylor expansion $f(x) = \sum_{n=0}^{\infty} c_n x^n$, a common method is to define

$$f(\hat{Q}) := \sum_{n=0}^{\infty} c_n \hat{Q}^n, \quad f(\boldsymbol{Q}) := \sum_{n=0}^{\infty} c_n \boldsymbol{Q}^n.$$

If $\boldsymbol{Q}_{k',k} = \langle a_{k'}|\hat{Q}|a_k\rangle$ *for an an orthonormal basis* $\{|a_k\rangle\}_k$*, show that*

$$\hat{Q} = \sum_{k',k} |a_{k'}\rangle\boldsymbol{Q}_{k',k}\langle a_k| \quad \Rightarrow \quad f(\hat{Q}) = \sum_{k',k} |a_{k'}\rangle\big(f(\boldsymbol{Q})\big)_{k',k}\langle a_k|. \tag{1}$$

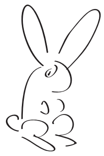
Hint: Beware of the difference between the operator $\hat{Q}$ and the matrix $\boldsymbol{Q}$. Also, there was a reason for why we bothered to do c). **(2 points)**

[1] It is quite common in the literature to put hats on operators, but we won't use this in a consistent manner in this course.

e) A particularly useful special case of (1) is if $\{|a_k\rangle\}_k$ diagonalizes $\hat{Q}$, i.e., that $\hat{Q} = \sum_k |a_k\rangle q_k \langle a_k|$ for some (possibly complex) numbers q_k. *Show that in this case*

$$f(\hat{Q}) = \sum_k |a_k\rangle f(q_k)\langle a_k|. \tag{2}$$

Hint: There is more than one route to show this, but you could think of how the matrix representation $\boldsymbol{Q}$ looks like in this case, and then how $\boldsymbol{Q}^n$ looks like. **(2 points)**



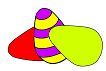
Remark: For operators that have an eigenvalue decomposition, (2) can be regarded as an alternative definition of $f(\hat{Q})$.

2 The position and momentum representations

Let $\{|\vec{x}\rangle\}_{\vec{x}\in\mathbb{R}^3}$ be joint 'eigenstates' of the position operators $\hat{\vec{X}} = (\hat{X}_1, \hat{X}_2, \hat{X}_3)$, i.e., $\hat{\vec{X}}|\vec{x}\rangle = \vec{x}|\vec{x}\rangle$. Analogously, let $\{|\vec{k}\rangle\}_{\vec{k}\in\mathbb{R}^3}$ be joint 'eigenstates' of the momentum operators $\hat{\vec{P}} = (\hat{P}_1, \hat{P}_2, \hat{P}_3)$. For these objects we have the orthonormality relations and resolutions of identity

$$\langle\vec{x}'|\vec{x}\rangle = \delta(\vec{x}' - \vec{x}), \quad \int |\vec{x}\rangle\langle\vec{x}|d^3x = \hat{1},$$

$$\langle\vec{k}'|\vec{k}\rangle = \delta(\vec{k}' - \vec{k}), \quad \int |\vec{k}\rangle\langle\vec{k}|d^3k = \hat{1}.$$



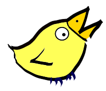
a) *Use the resolution of identity to show that an operator $\hat{Q}$ and its position representation $Q(\vec{x}', \vec{x}) = \langle\vec{x}'|\hat{Q}|\vec{x}\rangle$ are related as*

$$\hat{Q} = \int\int Q(\vec{x}', \vec{x})|\vec{x}'\rangle\langle\vec{x}|d^3x' d^3x.$$

(1 point)

b) *Determine the momentum representation $\vec{P}(\vec{k}', \vec{k}) = \langle\vec{k}'|\hat{\vec{P}}|\vec{k}\rangle$ of the momentum operator $\hat{P}$.* **(1 point)**

Remark: Note that $\hat{\vec{P}} = (\hat{P}_1, \hat{P}_2, \hat{P}_3)$ is a vector-operator, and as a consequence $\vec{P}(\vec{k}', \vec{k})$ is vector-valued function. This can be compared with $\hat{Q}$ in a) which only is a single operator, with the consequence that $Q(\vec{x}', \vec{x})$ is a scalar function.



c) Assume that

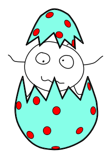
$$\langle\vec{x}|\vec{k}\rangle = (2\pi)^{-3/2} e^{i\vec{k}\cdot\vec{x}}. \tag{3}$$

Express the position representation $\vec{P}(\vec{x}', \vec{x}) = \langle\vec{x}'|\hat{\vec{P}}|\vec{x}\rangle$ in terms of the momentum representation $\vec{P}(\vec{k}', \vec{k})$. Next, insert the result in b) to express $\vec{P}(\vec{x}', \vec{x})$ as an integral over $\vec{k}$. **(3 points)**

d) *Use* (3) to show that

$$\delta(\vec{x}' - \vec{x}) = (2\pi)^{-3} \int e^{i\vec{k}(\vec{x}' - \vec{x})} d^3k.$$

(2 points)



e) *Show that*

$$\langle\vec{x}'|\hat{\vec{P}}|\psi\rangle = -i\vec{\nabla}_{\vec{x}'}\psi(\vec{x}'), \tag{4}$$

for $\psi(\vec{x}') = \langle\vec{x}'|\psi\rangle$. **(3 points)**

Remark: In textbooks one can sometimes see identifications of the form "$\hat{\vec{P}} \equiv -i\vec{\nabla}$". Equation (4) can be regarded as a formalization of that claim. In words, (4) in essence says that the action of the momentum operator $\hat{\vec{P}}$ on a state $|\psi\rangle$ gets translated into the action of the differential operator $-i\vec{\nabla}$ on the position representation $\psi(\vec{x})$ of that state. In other words, "$\hat{P}$ acts like $-i\vec{\nabla}$" in the position representation.