Física Quântica I / Mecânica Quântica (2021/22)

Folha de Problemas 2 (kets, bras, operadores)

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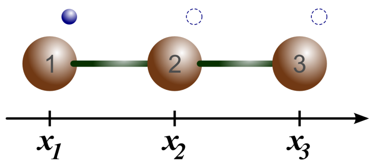
— Soluções —

Problema 1 | Representação e ação de operadores lineares

Considere o sistema físico que consiste num eletrão que, em cada momento, pode ocupar um dos três átomos de uma molécula. O conjunto $\{|x_1\rangle, |x_2\rangle, |x_3\rangle\}$ define uma base ortonormal do espaço de estados $\mathbb{V}^3(\mathbb{C})$ deste eletrão, onde x_i se refere à posição de cada átomo.



Nesse espaço, o operador $\hat{\mathrm{R}}$ é definido pela sua ação nos kets da base segundo:

$$\hat{\mathrm{R}}|x_1\rangle = i|x_2\rangle, \qquad \hat{\mathrm{R}}|x_2\rangle = i|x_3\rangle, \qquad \hat{\mathrm{R}}|x_3\rangle = i|x_1\rangle.$$

Suponha que o vetor de estado do sistema é dado por

$$|\psi\rangle = \frac{1}{\sqrt{5}}|x_1\rangle + \frac{1+i}{\sqrt{5}}|x_2\rangle + \frac{1-i}{\sqrt{5}}|x_3\rangle.$$

1. Escreva a matriz que representa o operador $\hat{\mathrm{R}}$ na base especificada acima.

2. Mostre que o operador $\hat{\mathrm{R}}$ se pode escrever como

$$\hat{\mathrm{R}} = i|x_2\rangle\langle x_1| + i|x_3\rangle\langle x_2| + i|x_1\rangle\langle x_3|.$$

3. Este operador $\hat{\mathrm{R}}$ é Hermítico?

4. Calcule $\hat{\mathrm{R}}|\psi\rangle$ e $\langle\psi|\hat{\mathrm{R}}$.

5. Calcule o valor esperado de $\hat{\mathrm{R}}$ no estado ψ, ou seja, determine $\langle\psi|\hat{\mathrm{R}}|\psi\rangle$.

6. Calcule a representação matricial do operador $\hat{\rho} \equiv |\psi\rangle\langle\psi|$ na base $\{|x_i\rangle\}$.

7. O operador $\hat{\rho}$ é Hermítico?

8. Mostre que

$$\langle\psi|\hat{\mathrm{R}}|\psi\rangle = \mathrm{Tr}\left(\hat{\mathrm{R}}\,\hat{\rho}\right).$$

   [*Aqui, Tr*$(\hat{\mathrm{A}})$ *significa o traço do operador* $\hat{\mathrm{A}}$*, que se obtém calculando o traço da matriz que o representa.*]

Solution

Since we are given how the operator acts on the basis vectors, its matrix elements are obtained immediately from the definition

$$R_{ij} \equiv \langle x_i|\hat{\mathrm{R}}|x_j\rangle.$$

1. Its matrix representation is thus

$$R = \begin{bmatrix} 0 & 0 & i \\ i & 0 & 0 \\ 0 & i & 0 \end{bmatrix}.$$

2. We saw in the lectures that every operator can be written in terms of its matrix elements in a given basis as

$$\hat{\mathrm{R}} = \sum_{i,j} R_{ij}|x_i\rangle\langle x_j|.$$

In the specific case of the given operator, we found in the previous question that the only non-zero matrix elements are R_{13}, R_{21}, and R_{32}, which are all equal to i. Consequently, we have

$$\begin{aligned}\hat{\mathrm{R}} = \sum_{i=1}^{3}\sum_{j=1}^{3} R_{ij}|x_i\rangle\langle x_j| &= R_{13}|x_1\rangle\langle x_3| + R_{21}|x_2\rangle\langle x_1| + R_{32}|x_3\rangle\langle x_2| + 0 + \cdots + 0 \\ &= i|x_2\rangle\langle x_1| + i|x_3\rangle\langle x_2| + i|x_1\rangle\langle x_3|.\end{aligned}$$

Alternative approach. In the particular case of this problem, we don't necessarily need to use the matrix representation of $\hat{\mathrm{R}}$ to show whether the given ket-bra expansion of $\hat{\mathrm{R}}$ is correct, because we already know the action of $\hat{\mathrm{R}}$ on all the basis vectors. As stated at the beginning of the problem text:

$$\hat{\mathrm{R}}|x_1\rangle = i|x_2\rangle, \qquad \hat{\mathrm{R}}|x_2\rangle = i|x_3\rangle, \qquad \hat{\mathrm{R}}|x_3\rangle = i|x_1\rangle. \tag{1.1}$$

Since this initial specification defines the operator $\hat{\mathrm{R}}$ completely, we can verify whether the given form,

$$\hat{\mathrm{R}} = i|x_2\rangle\langle x_1| + i|x_3\rangle\langle x_2| + i|x_1\rangle\langle x_3|, \tag{1.2}$$

is correct or not by simply applying it to the 3 basis vectors. Starting with $|x_1\rangle$:

$$\begin{aligned}\hat{\mathrm{R}}|x_1\rangle &= \Big(i|x_2\rangle\langle x_1| + i|x_3\rangle\langle x_2| + i|x_1\rangle\langle x_3|\Big)\,|x_1\rangle \\ &= i|x_2\rangle\langle x_1|x_1\rangle + i|x_3\rangle\langle x_2|x_1\rangle + i|x_1\rangle\langle x_3|x_1\rangle \\ &= i|x_2\rangle\delta_{11} + i|x_3\rangle\cancelto{0}{\delta_{21}} + i|x_1\rangle\cancelto{0}{\delta_{31}} \\ &= i|x_2\rangle\end{aligned}$$

Repeating the procedure for $|x_2\rangle$ and $|x_3\rangle$:

$$\begin{aligned}\hat{\mathrm{R}}|x_2\rangle &= \Big(i|x_2\rangle\langle x_1| + i|x_3\rangle\langle x_2| + i|x_1\rangle\langle x_3|\Big)\,|x_2\rangle \\ &= i|x_2\rangle\cancelto{0}{\langle x_1|x_2\rangle} + i|x_3\rangle\cancelto{1}{\langle x_2|x_2\rangle} + i|x_1\rangle\cancelto{0}{\langle x_3|x_2\rangle} \\ &= i|x_2\rangle,\end{aligned}$$

$$
\begin{aligned}
\hat{\mathrm{R}}|x_3\rangle &= \Big(i|x_2\rangle\langle x_1| + i|x_3\rangle\langle x_2| + i|x_1\rangle\langle x_3|\Big)\,|x_3\rangle \\
&= i|x_2\rangle\cancelto{0}{\langle x_1|x_3\rangle} + i|x_3\rangle\cancelto{0}{\langle x_2|x_3\rangle} + i|x_1\rangle\cancelto{1}{\langle x_3|x_3\rangle} \\
&= i|x_1\rangle.
\end{aligned}
$$

Since we obtained exactly the same results as in eq. (1.1), we conclude that eq. (1.2) indeed provides the correct expansion of $\hat{\mathrm{R}}$ in terms of basis ket-bras.

3. If the operator is Hermitian it should be represented by an Hermitian matrix. Let's calculate the Hermitian conjugate of the matrix we found above for $\hat{\mathrm{R}}$:

$$
R^\dagger = \begin{bmatrix} 0 & -i & 0 \\ 0 & 0 & -i \\ -i & 0 & 0 \end{bmatrix}
$$

Since $R^\dagger \neq R$ the operator is *not* Hermitian.

Another way to see this is from the definition of the operator in the "ket-bra" form:

$$
\hat{\mathrm{R}} = i|x_2\rangle\langle x_1| + i|x_3\rangle\langle x_2| + i|x_1\rangle\langle x_3|.
$$

When we take its Hermitian conjugate (transpose + conjugate) we obtain

$$
\hat{\mathrm{R}}^\dagger = -i|x_1\rangle\langle x_2| - i|x_2\rangle\langle x_3| - i|x_3\rangle\langle x_1|,
$$

from where we conclude that $\hat{\mathrm{R}} \neq \hat{\mathrm{R}}^\dagger$, and therefore it is not Hermitian.

4. The given state vector ψ is

$$
|\psi\rangle = \frac{1}{\sqrt{5}}|x_1\rangle + \frac{1+i}{\sqrt{5}}|x_2\rangle + \frac{1-i}{\sqrt{5}}|x_3\rangle.
$$

The action of $\hat{\mathrm{R}}$ on it is straightforward to obtain, by directly applying how $\hat{\mathrm{R}}$ acts on each of the basis kets:

$$
\begin{aligned}
\hat{\mathrm{R}}|\psi\rangle &= \frac{1}{\sqrt{5}}\,\hat{\mathrm{R}}|x_1\rangle + \frac{1+i}{\sqrt{5}}\,\hat{\mathrm{R}}|x_2\rangle + \frac{1-i}{\sqrt{5}}\,\hat{\mathrm{R}}|x_3\rangle \\
&= \frac{1}{\sqrt{5}}\,(i|x_2\rangle) + \frac{1+i}{\sqrt{5}}\,(i|x_3\rangle) + \frac{1-i}{\sqrt{5}}\,(i|x_1\rangle) \\
&= \frac{i+1}{\sqrt{5}}|x_1\rangle + \frac{i}{\sqrt{5}}|x_2\rangle + \frac{i-1}{\sqrt{5}}|x_3\rangle.
\end{aligned}
$$

For the calculation of $\langle\psi|\hat{\mathrm{R}}$, we can begin by noting that we can write

$$
\langle\psi|\hat{\mathrm{R}} = \left(\hat{\mathrm{R}}^\dagger|\psi\rangle\right)^\dagger.
$$

So, one option is to use the definition for $\hat{\mathrm{R}}^\dagger$ derived above

$$
\hat{\mathrm{R}}^\dagger = -i|x_1\rangle\langle x_2| - i|x_2\rangle\langle x_3| - i|x_3\rangle\langle x_1|,
$$

and calculate $\hat{\mathrm{R}}^\dagger|\psi\rangle$. Doing that explicitly, we obtain:

$$\begin{aligned}
\hat{\mathrm{R}}^\dagger|\psi\rangle &= (-i|x_1\rangle\langle x_2| - i|x_2\rangle\langle x_3| - i|x_3\rangle\langle x_1|)\left(\frac{1}{\sqrt{5}}|x_1\rangle + \frac{1+i}{\sqrt{5}}|x_2\rangle + \frac{1-i}{\sqrt{5}}|x_3\rangle\right)\\
&= \frac{-i}{\sqrt{5}}\left(|x_1\rangle\langle x_2| + |x_2\rangle\langle x_3| + |x_3\rangle\langle x_1|\right)|x_1\rangle\\
&\quad + \frac{1-i}{\sqrt{5}}\left(|x_1\rangle\langle x_2| + |x_2\rangle\langle x_3| + |x_3\rangle\langle x_1|\right)|x_2\rangle\\
&\quad + \frac{-1-i}{\sqrt{5}}\left(|x_1\rangle\langle x_2| + |x_2\rangle\langle x_3| + |x_3\rangle\langle x_1|\right)|x_3\rangle\\
\\
&= \frac{-i}{\sqrt{5}}\left(|x_1\rangle\langle x_2|x_1\rangle + |x_2\rangle\langle x_3|x_1\rangle + |x_3\rangle\langle x_1|x_1\rangle\right)\\
&\quad + \frac{1-i}{\sqrt{5}}\left(|x_1\rangle\langle x_2|x_2\rangle + |x_2\rangle\langle x_3|x_2\rangle + |x_3\rangle\langle x_1|x_2\rangle\right)\\
&\quad + \frac{-1-i}{\sqrt{5}}\left(|x_1\rangle\langle x_2|x_3\rangle + |x_2\rangle\langle x_3|x_3\rangle + |x_3\rangle\langle x_1|x_3\rangle\right)\\
\\
&= \frac{-i}{\sqrt{5}}|x_3\rangle + \frac{1-i}{\sqrt{5}}|x_1\rangle + \frac{-1-i}{\sqrt{5}}|x_2\rangle\\
&= \frac{1-i}{\sqrt{5}}|x_1\rangle + \frac{-1-i}{\sqrt{5}}|x_2\rangle + \frac{-i}{\sqrt{5}}|x_3\rangle.
\end{aligned}$$

And finally,

$$\langle\psi|\hat{\mathrm{R}} = \left(\hat{\mathrm{R}}^\dagger|\psi\rangle\right)^\dagger = \frac{1+i}{\sqrt{5}}\langle x_1| + \frac{i-1}{\sqrt{5}}\langle x_2| + \frac{i}{\sqrt{5}}\langle x_3|.$$

Alternative approach. A faster way to calculate the bra $\langle\psi|\hat{\mathrm{R}}$ is to use the matrix representation of both the bra and the operator (because we already know them from the previous questions), and multiply the two matrices in the same order:

$$\langle\psi|\hat{\mathrm{R}} \qquad \longrightarrow \qquad \begin{bmatrix}\frac{1}{\sqrt{5}} & \frac{1-i}{\sqrt{5}} & \frac{1+i}{\sqrt{5}}\end{bmatrix}\begin{bmatrix}0 & 0 & i\\ i & 0 & 0\\ 0 & i & 0\end{bmatrix} = \begin{bmatrix}i\frac{1-i}{\sqrt{5}} & i\frac{1+i}{\sqrt{5}} & \frac{i}{\sqrt{5}}\end{bmatrix} = \begin{bmatrix}\frac{i+1}{\sqrt{5}} & \frac{i-1}{\sqrt{5}} & \frac{i}{\sqrt{5}}\end{bmatrix}.$$

This row representation means that

$$\langle\psi|\hat{\mathrm{R}} = \frac{1+i}{\sqrt{5}}\langle x_1| + \frac{i-1}{\sqrt{5}}\langle x_2| + \frac{i}{\sqrt{5}}\langle x_3|.$$

5. From the results obtained above, the expectation value is given by

$$\begin{aligned}
\langle\psi|\left(\hat{\mathrm{R}}|\psi\rangle\right) &= \left(\frac{1}{\sqrt{5}}\langle x_1| + \frac{1-i}{\sqrt{5}}\langle x_2| + \frac{1+i}{\sqrt{5}}\langle x_3|\right)\left(\frac{i+1}{\sqrt{5}}|x_1\rangle + \frac{i}{\sqrt{5}}|x_2\rangle + \frac{i-1}{\sqrt{5}}|x_3\rangle\right)\\
&= \left(\frac{1}{\sqrt{5}}\right)\left(\frac{i+1}{\sqrt{5}}\right) + \left(\frac{1-i}{\sqrt{5}}\right)\left(\frac{i}{\sqrt{5}}\right) + \left(\frac{1+i}{\sqrt{5}}\right)\left(\frac{i-1}{\sqrt{5}}\right)\\
&= \frac{2i}{5}
\end{aligned}$$

6. According to the definition, the matrix elements ρ_{ij} of $\hat{\rho}$ should be given by

$$\rho_{ij} = \langle x_i|\hat{\rho}|x_j\rangle = \langle x_i|\Big(|\psi\rangle\langle\psi|\Big)|x_j\rangle = \langle x_i|\psi\rangle\langle\psi|x_j\rangle.$$

We now recall that the number $\langle x_i|\psi\rangle$ is simply the projection of $|\psi\rangle$ along the basis ket $|x_i\rangle$, so that we can immediately write

$$\langle x_1|\psi\rangle = \tfrac{1}{\sqrt{5}}, \quad \langle x_2|\psi\rangle = \tfrac{1+i}{\sqrt{5}}, \quad \langle x_3|\psi\rangle = \tfrac{1-i}{\sqrt{5}}.$$

And, since $\langle\psi|x_i\rangle = \langle x_i|\psi\rangle^*$, we have

$$\langle\psi|x_1\rangle = \tfrac{1}{\sqrt{5}}, \quad \langle\psi|x_2\rangle = \tfrac{1-i}{\sqrt{5}}, \quad \langle\psi|x_3\rangle = \tfrac{1+i}{\sqrt{5}}.$$

Combining the different pairs of products involving $\langle x_i|\psi\rangle$ and $\langle\psi|x_j\rangle$, the matrix representation of $\hat{\rho}$ becomes

$$\hat{\rho} = |\psi\rangle\langle\psi| \quad \mapsto \quad \frac{1}{5}\begin{bmatrix} 1 & 1-i & 1+i \\ 1+i & 2 & 2i \\ 1-i & -2i & 2 \end{bmatrix}.$$

Note: An equivalent way of obtaining the matrix representation of this operator is to consider the column and row representations of $|\psi\rangle$ and $\langle\psi|$, respectively, and compute their product in the same order as that in which the ket and bra appear in the definition of the operator, i.e.,

$$|\psi\rangle\langle\psi| \quad \mapsto \quad \begin{bmatrix} \frac{1}{\sqrt{5}} \\ \frac{1+i}{\sqrt{5}} \\ \frac{1-i}{\sqrt{5}} \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{5}} & \frac{1-i}{\sqrt{5}} & \frac{1+i}{\sqrt{5}} \end{bmatrix} = \frac{1}{5}\begin{bmatrix} 1 & 1-i & 1+i \\ 1+i & 2 & 2i \\ 1-i & -2i & 2 \end{bmatrix}.$$

7. We can see that it is Hermitian because, when we compute its Hermitian conjugate, we get

$$(|\psi\rangle\langle\psi|)^\dagger = (\langle\psi|)^\dagger\,(|\psi\rangle)^\dagger = |\psi\rangle\langle\psi|,$$

where we used the fact that, when performing the Hermitian conjugation of a product we must reverse the order of the terms:

$$(\hat{\mathrm{A}}\,\hat{\mathrm{B}})^\dagger = \hat{\mathrm{B}}^\dagger\hat{\mathrm{A}}^\dagger.$$

Since $\big(|\psi\rangle\langle\psi|\big)^\dagger = |\psi\rangle\langle\psi|$, this operator is Hermitian. (Equivalently, we can see that the operator is Hermitian because its matrix representation, computed in the previous question, is an Hermitian matrix.)

8. We must compute the trace of the product of the two operators $\hat{\mathrm{R}}$ and $|\psi\rangle\langle\psi|$. To do that, we compute the product of the respective matrices and calculate the trace of the resulting matrix. (Recall that the trace of a matrix is the sum of its diagonal elements.) Taking the matrices found in questions 1 and 6 above,

$$\begin{aligned} \hat{\mathrm{R}}\,\hat{\rho} \quad \mapsto \quad & \frac{1}{5}\begin{bmatrix} 0 & 0 & i \\ i & 0 & 0 \\ 0 & i & 0 \end{bmatrix}\begin{bmatrix} 1 & 1-i & 1+i \\ 1+i & 2 & 2i \\ 1-i & -2i & 2 \end{bmatrix} \\ = & \frac{1}{5}\begin{bmatrix} i+1 & 2 & 2i \\ i & i+1 & i-1 \\ i-1 & 2i & -2 \end{bmatrix}. \end{aligned}$$

The trace of this matrix is given by the sum of its diagonal elements:

$$\mathrm{Tr}\left(\hat{\mathrm{R}}\,\hat{\rho}\right) = \frac{i+1}{5} + \frac{i+1}{5} - \frac{2}{5} = \frac{2i}{5}.$$

This is precisely the result obtained earlier in question 5. Hence, it is true that

$$\langle\psi|\hat{\mathrm{R}}|\psi\rangle = \mathrm{Tr}\left(\hat{\mathrm{R}}\,\hat{\rho}\right).$$