Física Quântica I / Mecânica Quântica (2021/22)

Folha de Problemas 7 (funções de onda nas bases de X e de P)

Vitor M. Pereira | Universidade do Minho | 5-Abr-2022

— Soluções —

Problema 1 | $\hat{\mathrm{X}}$ na base de $\hat{\mathrm{P}}$ e vice-versa

Usando apenas as identidades

$$\hat{P}|p\rangle = p\,|p\rangle, \qquad \hat{X}|x\rangle = x\,|x\rangle, \qquad \langle x|p\rangle = \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}},$$

onde $|p\rangle$ e $|x\rangle$ são, respetivamente, os auto-estados do operador momento e posição:

1. Mostre que os elementos de matriz de $\hat{P}$ na base de posição são dados por

$$\langle x|\hat{P}|x'\rangle = -i\hbar\,\frac{\partial}{\partial x}\delta\left(x-x'\right).$$

2. Mostre que os elementos de matriz de $\hat{X}$ na base de momento são dados por

$$\langle p|\hat{X}|p'\rangle = i\hbar\,\frac{\partial}{\partial p}\delta\left(p-p'\right).$$

3. Mostre que a ação de $\hat{X}$ sob funções de onda na base de momento é dada por

$$\langle p|\hat{X}|\psi\rangle = i\hbar\frac{\partial}{\partial p}\psi(p).$$

4. A regra geral para escrever a equação de Schrödinger na base de posição consiste em partir do Hamiltoniano clássico $\mathcal{H}(x,\,p)$ e convertê-lo num operador diferencial através das substituições.

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = \mathcal{H}\Big(x,\,p\to\frac{\hbar}{i}\frac{\partial}{\partial x}\Big)\,\psi(x,t).$$

   Usando os resultados das questões anteriores, escreva a regra correspondente que permite obter a equação de Schrödinger para as funções de onda da base do momento:

$$i\hbar\frac{\partial}{\partial t}\psi(p,t) = \mathcal{H}\Big(x\to ?,\,p\to ?\Big)\,\psi(p,t).$$

Sugestão — As relações de fecho

$$\mathbf{1} = \int dx\,|x\rangle\langle x|, \qquad \mathbf{1} = \int dp\,|p\rangle\langle p|$$

são úteis para as demonstrações acima. Pode também ser útil notar que

$$\int dx\,x\,e^{\alpha x} = \frac{\partial}{\partial\alpha}\left[\int dx\,e^{\alpha x}\right].$$

Solution

1. Since the action of $\hat{P}$ is trivial in the basis $|p\rangle$, we resort to the resolution of the identity in this basis,
$$\mathbf{1} = \int dp\, |p\rangle\langle p|,$$
to facilitate the calculation:
$$\langle x|\hat{P}|x'\rangle = \langle x|\hat{P}\left(\int dp|p\rangle\langle p|\right)|x'\rangle = \int dp\langle x|\hat{P}|p\rangle\langle p|x'\rangle = \int dp\, p\langle x|p\rangle\frac{e^{-ipx'/\hbar}}{\sqrt{2\pi\hbar}}$$
$$\Big\downarrow \text{ substitute } \langle x|p\rangle = \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}}$$
$$= \frac{1}{2\pi\hbar}\int dp\, p\, e^{ip(x-x')/\hbar} = \frac{\hbar}{i}\frac{\partial}{\partial x}\left[\frac{1}{2\pi\hbar}\int dp\, e^{ip(x-x')/\hbar}\right]$$
$$= \frac{\hbar}{i}\frac{\partial}{\partial x}\delta\left(x-x'\right) \qquad \boxdot$$
In the last step we used the integral representation of the Dirac-delta function:
$$\delta\left(x-x'\right) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{\pm k(x-x')}dk.$$
Note — We can confirm this result against what we derived in lectures, where we saw that
$$\langle x|\hat{P}|\psi\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x}\psi(x) = \frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|\psi\rangle.$$
Hence, we can directly obtain the result above by setting $|\psi\rangle = |x'\rangle$:
$$\langle x|\hat{P}|x'\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|x'\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x}\delta(x-x') = -i\hbar\delta'(x-x').$$

2. We do exactly as above, but resolving the identity now in the basis of $\hat{X}$:
$$\langle p|\hat{X}|p'\rangle = \langle p|\hat{X}\left(\int dx|x\rangle\langle x|\right)|p'\rangle = \int dx\langle p|\hat{X}|x\rangle\langle x|p'\rangle$$
$$= \int dx\, x\langle p|x\rangle\frac{e^{ip'x/\hbar}}{\sqrt{2\pi\hbar}} = \frac{1}{2\pi\hbar}\int dx\, x\, e^{-ix(p-p')/\hbar}$$
$$= -\frac{\hbar}{i}\frac{\partial}{\partial p}\left[\frac{1}{2\pi\hbar}\int dx\, e^{-ix(p-p')/\hbar}\right]$$
$$= -\frac{\hbar}{i}\frac{\partial}{\partial p}\delta\left(p-p'\right) \qquad \boxdot$$

3. Similarly to the previous question, we want to insert a resolution of the identity that makes the action of $\hat{X}$ as simple as possible. In this case it is simply
$$\langle p|\hat{X}|\psi\rangle = \langle p|\left(\int dx|x\rangle\langle x|\right)\hat{X}|\psi\rangle = \int dx\, x\langle p|x\rangle\langle x|\psi\rangle.$$

Now, since we want to express the result in terms of $\psi(p)$ rather than $\psi(r)$ we insert another identity in $\langle x|\psi\rangle$ to make the momentum wavefunction $\psi(p)$ appear in the expression:

$$\langle p|\hat{X}|\psi\rangle = \int dx\, x\langle p|x\rangle\langle x|\psi\rangle = \int dx \int dp'\, x\langle p|x\rangle\langle x|p'\rangle\langle p'|\psi\rangle$$

$$\Big\downarrow \text{ substitute } \langle x|p'\rangle = \frac{e^{ip'x/\hbar}}{\sqrt{2\pi\hbar}} \text{ and } \langle p|x\rangle = \langle x|p\rangle^* = \frac{e^{-ipx/\hbar}}{\sqrt{2\pi\hbar}}$$

$$= \int dp'\, \psi(p') \int dx\, x \frac{e^{i(p'-p)x/\hbar}}{2\pi\hbar}.$$

We note that this integral over x is close to the definition of the Dirac delta function, except for the factor x that multiplies the exponential function. If we use the identity provided in the suggestion to this problem,

$$\int dx\, x\, e^{\alpha x} = \frac{\partial}{\partial\alpha}\left[\int dx\, e^{\alpha x}\right],$$

we can express the previous result as

$$\begin{aligned}\langle p|\hat{X}|\psi\rangle &= \frac{1}{2\pi\hbar}\int dp'\psi(p')\left(-\frac{\hbar}{i}\frac{\partial}{\partial p}\int dx\, x\, e^{i(p'-p)x/\hbar}\right)\\ &= -\frac{\hbar}{i}\int dp'\psi(p')\left[\frac{\partial}{\partial p}\delta\left(p-p'\right)\right] = i\hbar\frac{\partial}{\partial p}\int dp'\psi(p')\delta\left(p-p'\right)\\ &= i\hbar\frac{\partial}{\partial p}\,\psi(p) \qquad \boxdot\end{aligned}$$

Alternative approach. You might notice that, if we expand $|\psi\rangle$ in the momentum eigenbasis,

$$|\psi\rangle = \int dp'\, \psi(p')\, |p'\rangle,$$

the projection $\langle p|\hat{X}|\psi\rangle$ becomes

$$\langle p|\hat{X}|\psi\rangle = \int dp'\, \psi(p')\, \langle p|\hat{X}|p'\rangle,$$

and we can directly use the result derived in the previous question. That would lead us to

$$\langle p|\hat{X}|\psi\rangle = \int dp'\, \psi(p')\, \langle p|\hat{X}|p'\rangle = i\hbar\int dp'\, \psi(p')\, \left[\frac{\partial}{\partial p}\delta\left(p-p'\right)\right].$$

Note that in the last result we have an integration over the variable p' and a derivative with respect to another, independent, variable p. Hence, the $\frac{\partial}{\partial p}$ can be put outside the integral *because nothing else in the integrand depends on* p:

$$\langle p|\hat{X}|\psi\rangle = i\hbar\frac{\partial}{\partial p}\left[\int dp'\, \psi(p')\, \delta\left(p-p'\right)\right] = i\hbar\frac{\partial\psi(p)}{\partial p}.$$

This is the same as derived above, of course.

4. From the result of the previous question we can extract the action of any function of the position in the momentum wavefunctions:

$$\langle p|V(\hat{X})|\psi\rangle = V\left(i\hbar\frac{\partial}{\partial p}\right)\psi(p).$$

The expression on the right-hand side means the following: *"take the function that defines the potential energy as a function of position, replace $V(x)$ by its Taylor expansion, replace $x \to i\hbar\partial/\partial p$ as the argument of that expansion."*

This is all we need to write the Schrodinger equation in the momentum basis:

$$\begin{aligned}
& i\hbar\frac{d}{dt}|\psi(t)\rangle = \hat{H}(\hat{X},\hat{P})|\psi(t)\rangle \\
\Leftrightarrow\quad & i\hbar\frac{d}{dt}\langle p|\psi(t)\rangle = \langle p|\hat{H}(\hat{X},\hat{P})|\psi(t)\rangle \\
\Leftrightarrow\quad & i\hbar\frac{d}{dt}\psi(p,t) = \frac{1}{2m}\langle p|\hat{P}^2|\psi(t)\rangle + \langle p|V(\hat{X})|\psi(t)\rangle \\
\Leftrightarrow\quad & i\hbar\frac{d}{dt}\psi(p,t) = \frac{p^2}{2m}\langle p|\psi(p,t)\rangle + V\left(i\hbar\frac{\partial}{\partial p}\right)\psi(p) \\
\Leftrightarrow\quad & i\hbar\frac{d}{dt}\psi(p,t) = \frac{p^2}{2m}\psi(p,t) + V\left(i\hbar\frac{\partial}{\partial p}\right)\psi(p).
\end{aligned}$$

We see from above that the rule in momentum representation is simply to replace

$$x \to i\hbar\frac{\partial}{\partial p}$$

in the classical Hamiltonian function and convert the result into an operator that acts on the wavefunction $\psi(p)$. Therefore, to write the S.E. in the momentum basis we start from the classical Hamiltonian and apply that replacement

$$\mathcal{H}(x,\,p) \quad \xrightarrow{x\to i\hbar\frac{\partial}{\partial p}} \quad i\hbar\frac{\partial}{\partial t}\psi(p,t) = \mathcal{H}\Big(i\hbar\frac{\partial}{\partial p},\,p\Big)\,\psi(p,t).$$

The object $\mathcal{H}\Big(i\hbar\frac{\partial}{\partial p},\,p\Big)$ in the right-hand side is now a differential operator that acts on the momentum wavefunction $\psi(p)$.

Problema 2 | Normalizações

Determine a constante $\mathcal{N}$ que normaliza cada uma das seguintes funções de onda em todo o eixo real de x (assuma que $\lambda > 0$ em todas elas):

1. $\psi(x) = \mathcal{N}\,e^{-\lambda|x|}$.

2. $\psi(x) = \mathcal{N}\,e^{-\lambda x^2}$.

3. $\psi(x) = \mathcal{N}\,x\,e^{-\lambda x^2}$.

Nota — Os integrais Gaussianos podem ser obtidos através das relações seguintes, válidas quando $\mathrm{Re}\,\alpha > 0$:

$$I_0(\alpha) \equiv \int_{-\infty}^{+\infty} e^{-\alpha x^2} dx = \sqrt{\frac{\pi}{\alpha}}, \qquad I_{2n}(\alpha) \equiv \int_{-\infty}^{+\infty} x^{2n} e^{-\alpha\, x^2} dx = (-1)^n \frac{\partial^n}{\partial \alpha^n} I_0(\alpha),$$

$$I_{2n+1}(\alpha) \equiv \int_{-\infty}^{+\infty} x^{2n+1} e^{-\alpha\, x^2} dx = 0.$$

Solution

1. The normalization condition is
$$\int_{-\infty}^{+\infty} |\psi(x)|^2 \, dx = 1.$$
Imposing this condition on the given wavefunction we have:
$$1 = \int_{-\infty}^{+\infty} |\psi(x)|^2 \, dx = \mathcal{N}^2 \int_{-\infty}^{+\infty} e^{-2\lambda|x|} dx = 2\,\mathcal{N}^2 \int_0^{+\infty} e^{-2\lambda x} dx = 2\,\mathcal{N}^2 \,\frac{1}{2\lambda}.$$
Solving for $\mathcal{N}$ we get
$$\mathcal{N} = \sqrt{\lambda},$$
and the normalized wavefunction is therefore
$$\psi(x) = \sqrt{\lambda}\, e^{-\lambda|x|}.$$

2. In this case we will need to use one of the Gaussian integrals listed at the end of the problem text:
$$1 = \int_{-\infty}^{+\infty} |\psi(x)|^2 \, dx = \mathcal{N}^2 \int_{-\infty}^{+\infty} e^{-2\lambda x^2} dx = \mathcal{N}^2 \sqrt{\frac{\pi}{2\lambda}} \quad \longrightarrow \quad \mathcal{N} = \left(\frac{2\lambda}{\pi}\right)^{\frac{1}{4}}.$$
The normalized wavefunction is
$$\psi(x) = \left(\frac{2\lambda}{\pi}\right)^{\frac{1}{4}} e^{-\lambda x^2}.$$

3. When we impose the normalization condition we get
$$1 = \int_{-\infty}^{+\infty} |\psi(x)|^2 \, dx = \mathcal{N}^2 \int_{-\infty}^{+\infty} x^2 e^{-2\lambda x^2} dx. \qquad (*)$$
This integral has the form of the integral $I_{2n}(a)$ (provided at the end of the problem text) with $n = 1$:
$$I_2(a) = \int_{-\infty}^{+\infty} x^2 e^{-ax^2} dx.$$
Using the formula provided to evaluate $I_{2n}(\alpha)$ in terms of $I_0(\alpha)$, we obtain
$$I_2(\alpha) = -\frac{\partial}{\partial \alpha}\left[\int_{-\infty}^{+\infty} e^{-\alpha x^2} dx\right] = -\frac{\partial}{\partial \alpha}\sqrt{\frac{\pi}{\alpha}} = \frac{\sqrt{\pi}}{2\alpha^{3/2}}.$$

Adapting this to the integral we have in eq. (*) above, we finally conclude that

$$1 = \mathcal{N}^2 \frac{\sqrt{\pi}}{2\,(2\lambda)^{3/2}} \qquad \longrightarrow \qquad \mathcal{N} = 2\left(\frac{2\lambda^3}{\pi}\right)^{\frac{1}{4}}.$$

The normalized wavefunction is

$$\psi(x) = 2\left(\frac{2\lambda^3}{\pi}\right)^{\frac{1}{4}} x e^{-\lambda x^2}.$$

Problema 3 | Invocando simetria

A função de onda de uma partícula é dada por:

$$\psi(x) = \mathcal{N}\,\frac{e^{ikx}}{x^2 + a^2},$$

onde $\mathcal{N}$ é a constante de normalização. Calcule $\langle \hat{\mathrm{X}} \rangle$ e $\langle \hat{\mathrm{P}} \rangle$ neste estado.

Nota — Não calcule os integrais que encontrar explicitamente; analise antes a simetria do integrando, a qual, neste caso, permite determinar diretamente aqueles valores esperados.

Solution

For the expectation value of the position we have

$$\langle x \rangle = \int_{-\infty}^{+\infty} \psi^*(x)\; x\, \psi(x)\; dx = \int_{-\infty}^{+\infty} x\, |\psi(x)|^2\; dx = |\mathcal{N}|^2 \int_{-\infty}^{+\infty} \frac{x}{(x^2 + a^2)^2}\, dx = 0$$

The reason why this is zero is because the integrand consists of the product of an odd function and an even function, and the integration limits are symmetric with respect to the origin.

For the expectation value of the momentum we have

$$\langle p \rangle = \int_{-\infty}^{+\infty} \psi^*(x) \left(\frac{\hbar}{i}\frac{d}{dx}\right) \psi(x)\; dx$$

Now, the derivative under the integral is simply

$$\frac{d\psi(x)}{dx} = \mathcal{N}\left[\frac{ike^{ikx}}{x^2 + a^2} - \frac{2xe^{ikx}}{(x^2 + a^2)^2}\right] = \left[ik\psi(x) - \frac{2x}{x^2 + a^2}\psi(x)\right]$$

and so the expectation value becomes

$$\begin{aligned}
\langle p \rangle &= \frac{\hbar}{i}\int_{-\infty}^{+\infty} \left[ik\psi^*(x)\,\psi(x) - \frac{2x}{x^2 + a^2}\psi^*(x)\,\psi(x)\right] dx \\
&= \hbar k \int_{-\infty}^{+\infty} |\psi(x)|^2\, dx - \frac{2\hbar}{i}\int_{-\infty}^{+\infty} \frac{x}{x^2 + a^2}\, |\psi(x)|^2\, dx \\
&= \hbar k
\end{aligned}$$

where again the second term on the r.h.s. is zero by symmetry, and we used the fact that the wavefunction is assumed to be normalized to 1. Consequently, the final result is simply

$$\langle p \rangle = \hbar k.$$

Problema 4

Mostre que, para qualquer função de onda com a forma

$$\psi(x) = e^{ikx} f(x),$$

em que $f(x)$ é uma função *real* tal que $\psi(x)$ é uma função de quadrado integrável, se obtém

$$\langle \hat{P} \rangle = \hbar k.$$

Sugestão — Integre por partes e repare que, como $\psi(x)$ é de quadrado integrável, isso implica que $f(x) \xrightarrow{x \to \pm\infty} 0$.

Solution

Since we don't know whether the wavefunction is normalized or not, let us introduce, formally, the normalization constant

$$\mathcal{N} = \int |\psi(x)|^2 \, dx = \int [f(x)]^2 \, dx,$$

so that the wavefunction

$$\psi(x) = \frac{1}{\sqrt{\mathcal{N}}} e^{ikx} f(x)$$

is normalized to 1.

The expectation value of the momentum is calculated as

$$\langle \hat{P} \rangle = -\frac{i\hbar}{\mathcal{N}} \int \psi^*(x) \frac{d\psi(x)}{dx} \, dx = -\frac{i\hbar}{\mathcal{N}} \int \psi^*(x)\psi'(x) \, dx,$$

and

$$\psi'(x) = e^{ikx} \Big[ikf(x) + f'(x) \Big].$$

Therefore

$$\langle \hat{P} \rangle = \frac{\hbar k}{\mathcal{N}} \int [f(x)]^2 \, dx - i\hbar \int f(x) f'(x) \, dx. \qquad (\star)$$

The first term is simply $\hbar k$ because, as we saw in the first result above,

$$\int [f(x)]^2 \, dx = \mathcal{N}.$$

The second term is zero because

$$\begin{aligned} & \int f(x) f'(x) \, dx \overset{\text{(by parts)}}{=} \Big([f(x)]^2 \Big|_{-\infty}^{+\infty} - \int f(x) f'(x) \, dx \\ \Leftrightarrow \quad & 2 \int f(x) f'(x) \, dx = [f(+\infty)]^2 - [f(-\infty)]^2 = 0 \end{aligned}$$

since $f(x) \stackrel{x\to\pm\infty}{\longrightarrow} 0$ in order to make $\psi(x)$ square integrable. Consequently, only the first term of ($\star$) survives and the final result is

$$\langle\hat{P}\rangle = \hbar k \qquad \boxdot$$

Problema 5 | Um comutador prático

Mostre que, se dois operadores $\hat{A}$ e $\hat{B}$ obedecem à relação de comutação

$$\big[\hat{A},\, \hat{B}\big] = c, \qquad c \in \mathbb{Z}, \tag{5.1}$$

onde c é um número, então o seguinte é verdade para qualquer função $f(\cdot)$:

$$\big[\hat{A},\, f(\hat{B})\big] = c\, f'(\hat{B}) \qquad \text{e} \qquad \big[\hat{B},\, f(\hat{A})\big] = -c\, f'(\hat{A}), \tag{5.2}$$

onde f' representa a derivada de $f(\cdot)$ com respeito ao seu argumento.

Sugestão — (i) escreva a série de Taylor para $f(\hat{B})$; (ii) calcule o comutador de $\hat{A}$ com $\hat{B}^n$; (iii) use a identidade $[\hat{A}, \hat{B}\hat{C}] = \hat{B}[\hat{A}, \hat{C}] + [\hat{A}, \hat{B}]\hat{C}$ recursivamente até obter o comutador simples $[\hat{A}, \hat{B}]$; (iv) incorpore tudo na série de Taylor e interprete o que ela representa.

Nota — Como $\big[\hat{X},\, \hat{P}\big] = i\hbar$, o resultado acima é útil sempre que temos comutadores nos quais aparecem funções de $\hat{X}$ ou $\hat{P}$.

Solution

When dealing with a function of an operator, particularly in problems involving a generic function such as this, one should think in terms of the Taylor series that defines the function in question:

$$f(\hat{B}) = \sum_{n=0}^{\infty} f^{(n)}(0)\, \frac{\hat{B}^n}{n!}.$$

Calculating the commutators we want therefore requires the calculation of commutators of the type $\big[\hat{A}, \hat{B}^n\big]$. Recalling the identity (problem set 1)

$$\Big[\hat{R},\, \hat{S}\hat{W}\Big] = \hat{S}\,\Big[\hat{R},\, \hat{W}\Big] + \Big[\hat{R},\, \hat{S}\Big]\,\hat{W}$$

we can expand the commutator with powers of $\hat{B}$ as follows:

$$\Big[\hat{A}, \hat{B}^n\Big] = \Big[\hat{A}, \hat{B}\,\hat{B}^{n-1}\Big] = \hat{B}\,\Big[\hat{A}, \hat{B}^{n-1}\Big] + \Big[\hat{A}, \hat{B}\Big]\,\hat{B}^{n-1}.$$

In the case of interest here, the commutator $\big[\hat{A}, \hat{B}\big] = c\,\mathbf{1}$ with c a complex number. For this particular problem $c = i\hbar$, but let us keep it general and call it c. Hence, the equation above becomes

$$\Big[\hat{A}, \hat{B}^n\Big] = \hat{B}\,\Big[\hat{A}, \hat{B}^{n-1}\Big] + c\,\hat{B}^{n-1}.$$

The remaining commutator in the r.h.s. is exactly of the same type of the one one the l.h.s., so we can replace the result above recursively in the commutator on the r.h.s.:

$$\begin{aligned}
\left[\hat{A},\hat{B}^{n}\right] &= c\,\hat{B}^{n-1}+\hat{B}\left[\hat{A},\hat{B}^{n-1}\right]\\
&= c\,\hat{B}^{n-1}+\hat{B}\left\{c\,\hat{B}^{n-2}+\hat{B}\left[\hat{A},\hat{B}^{n-2}\right]\right\}\\
&= c\,\hat{B}^{n-1}+c\,\hat{B}^{n-1}+\hat{B}^{2}\left[\hat{A},\hat{B}^{n-2}\right]\\
&= 2c\,\hat{B}^{n-1}+\hat{B}^{2}\left[\hat{A},\hat{B}^{n-2}\right]\\
&= 2c\,\hat{B}^{n-1}+\hat{B}^{2}\left\{c\,\hat{B}^{n-3}+\hat{B}\left[\hat{A},\hat{B}^{n-3}\right]\right\}\\
&= 3c\,\hat{B}^{n-1}+\hat{B}^{3}\left[\hat{A},\hat{B}^{n-3}\right]\\
&\vdots\\
&\text{there is clearly a pattern here! Therefore,}\\
&\vdots\\
&= nc\,\hat{B}^{n-1}+\hat{B}^{n}\left[\hat{A},\hat{B}^{n-n}\right]\\
&= nc\,\hat{B}^{n-1}+\hat{B}^{n}\left[\hat{A},\mathbf{1}\right]\\
&= nc\,\hat{B}^{n-1}
\end{aligned}$$

This shows explicitly that $\left[\hat{A},\hat{B}^{n}\right]=nc\,\hat{B}^{n-1}$ (you can confirm that this is true by mathematical induction). Therefore the commutator with the function is

$$\begin{aligned}
\left[\hat{A},\,f(\hat{B})\right] &= \sum_{n=0}^{\infty}\frac{f^{(n)}(0)}{n!}\left[\hat{A},\hat{B}^{n}\right]=c\sum_{n=0}^{\infty}\frac{nf^{(n)}(0)}{n!}\hat{B}^{n-1}\\
&= c\sum_{n=1}^{\infty}\frac{f^{(n)}(0)}{(n-1)!}\hat{B}^{n-1}=c\sum_{n=0}^{\infty}\frac{f^{(n+1)}(0)}{n!}\hat{B}^{n}
\end{aligned}$$

(note the redefinition of the indices done in the last step). Since the last sum is the Taylor expansion for $f'(\hat{B})$ we have

$$\left[\hat{A},\,f(\hat{B})\right]=c\,f'(\hat{B})=i\hbar f'(\hat{B}) \qquad \boxdot$$

The demonstration of the second result would be completely analogous. But, in fact, we don't have to repeat it step by step again as we can simply use the result just obtained. Recalling that we defined $c=[\hat{A},\,\hat{B}]$, the last expression can be rewritten as

$$\left[\hat{A},\,f(\hat{B})\right]=\left[\hat{A},\,\hat{B}\right]f'(\hat{B})$$

and therefore, exchanging the roles of A, B, we get

$$\left[\hat{B},\,f(\hat{A})\right]=\left[\hat{B},\,\hat{A}\right]f'(\hat{A})=-i\hbar f'(\hat{A}) \qquad \boxdot$$

Problema 6 | Operador de translação

Recorrendo ao comutador canónico entre os operadores $\hat{X}$ e $\hat{P}$, e tendo em conta o resultado do problema anterior:

1. Calcule $\big[\hat{X},\, \hat{T}_a\big]$, onde $\hat{T}_a = e^{-ia\hat{P}/\hbar}$ é o operador de translação no espaço e $a \in \mathbb{R}$.
2. Mostre que $\hat{T}_a\,\hat{X}\,\hat{T}_a^\dagger = \hat{X} - a\hat{\mathbf{1}}$, onde $\hat{\mathbf{1}}$ é o operador identidade.

Solution

1. Since the position and momentum operators obey the commutation relation
$$[\hat{X}, \hat{P}] = i\hbar,$$
and since for any function $f(x)$ we know that
$$[\hat{X}, f(\hat{P})] = i\hbar f'(\hat{P}),$$
we conclude that
$$[\hat{X}, e^{-i\hat{P}a/\hbar}] = i\hbar\left(\frac{\partial}{\partial\hat{P}} e^{-i\hat{P}a/\hbar}\right) = a e^{-i\hat{P}a/\hbar} = a\hat{T}_a.$$

2. Since the right-hand side of $\hat{T}_a\,\hat{X}\,\hat{T}_a^\dagger = \hat{X} - a\hat{\mathbf{1}}$ does not have any translation operator, we must, somehow, manipulate the left-hand side to make them "disappear". One way to make the two operators $\hat{T}_a$ and $\hat{T}_a^\dagger$ "disappear" is by noting that $\hat{T}_a^\dagger \hat{T}_a = \hat{T}_a^{-1}\hat{T}_a = \mathbf{1}$, because $\hat{T}$ is a unitary operator (because $\hat{P}$ in the exponential is Hermitian). That entails swapping the placement of, for example, $\hat{X}$ and $\hat{T}_a$ which, since they don't commute as per the result of question (1), must be done by taking into account their commutator:
$$\hat{T}_a\,\hat{X} = \hat{X}\,\hat{T}_a + [\hat{T}_a, \hat{X}].$$
Using this replacement, we rewrite the left-hand side as follows:
$$\hat{T}_a\,\hat{X}\,\hat{T}_a^\dagger = \left(\hat{X}\,\hat{T}_a + [\hat{T}_a, \hat{X}]\right)\hat{T}_a^\dagger = \hat{X}\,\hat{T}_a\hat{T}_a^\dagger + [\hat{T}_a, \hat{X}]\hat{T}_a^\dagger = \hat{X} - a\hat{T}_a\,\hat{T}_a^\dagger = \hat{X} - a,$$
where in the last steps we used the fact that $\hat{T}_a$ is unitary and replaced $[\hat{T}_a, \hat{X}]$ by the result of (1) above.

Note — The result of question 2 means that the unitary transformation produced by $\hat{T}_a$ on the position operator indeed corresponds to a shift of $\hat{X}$ by the amount a. This explains why $\hat{T}_a$ is named "translation operator".

Problema 7 | Virial

Em física clássica, a quantidade designada *virial* de uma partícula que se move em 1D é definida como o produto da sua posição e do seu momento linear:
$$\mathcal{G}(x, p) \equiv xp.$$

1. Mostre que a tentativa de quantizar esta quantidade através da substituição habitual
$$\mathcal{G}(x \to \hat{X}, p \to \hat{P}) = \hat{X}\,\hat{P},$$
resulta num operador que não é uma observável.

2. Determine $\alpha \in \mathbb{R}$ de modo a que o operador definido alternativamente como

$$\hat{G} \equiv (1-\alpha)\,\hat{X}\,\hat{P} + \alpha \hat{P}\,\hat{X}$$

seja Hermítico. Este descreve adequadamente o virial em mecânica quântica.

3. Mostre que, se a partícula for descrita pelo Hamiltoniano clássico

$$\mathcal{H} = \frac{p^2}{2m} + V(x),$$

então, em qualquer estado ψ, verifica-se que

$$\frac{d\langle \hat{X}^2 \rangle_\psi}{dt} = \frac{2}{m}\langle \hat{G} \rangle_\psi, \qquad \text{onde} \qquad \langle \cdots \rangle_\psi \equiv \langle \psi | \cdots | \psi \rangle.$$

Solution

1. The operator $\hat{G}$ defined in this way is not Hermitian because

$$\left(\hat{G}\right)^\dagger = \left(\hat{X}\hat{P}\right)^\dagger = \hat{P}^\dagger \hat{X}^\dagger = \hat{P}\hat{X}$$

But since $\left[\hat{X}, \hat{P}\right] = i\hbar$, then

$$\left(\hat{G}\right)^\dagger = \hat{P}\hat{X} = \hat{X}\hat{P} - i\hbar \neq \hat{G}' \qquad \boxdot$$

2. In order for $\hat{G}$ to be Hermitian we must have

$$\begin{aligned}
\hat{G}^\dagger = \hat{G} \qquad &\Leftrightarrow \qquad \left[(1-\alpha)\,\hat{X}\,\hat{P} + \alpha \hat{P}\,\hat{X}\right]^\dagger = (1-\alpha)\,\hat{X}\,\hat{P} + \alpha \hat{P}\,\hat{X} \\
&\Leftrightarrow \qquad (1-\alpha)\,\hat{P}\hat{X} + \alpha \hat{X}\hat{P} = (1-\alpha)\,\hat{X}\,\hat{P} + \alpha \hat{P}\,\hat{X} \\
&\Leftrightarrow \qquad (1-\alpha)\left(\hat{P}\hat{X} - \hat{X}\,\hat{P}\right) + \alpha\left(\hat{X}\hat{P} - \hat{P}\,\hat{X}\right) = 0 \\
&\Leftrightarrow \qquad (1-\alpha)\left[\hat{P}, \hat{X}\right] + \alpha\left[\hat{X}, \hat{P}\right] = 0 \\
&\Leftrightarrow \qquad (1-\alpha)\,(-i\hbar) + \alpha i\hbar = 0 \\
&\Leftrightarrow \qquad \alpha = \frac{1}{2}
\end{aligned}$$

Therefore, the proper Hermitian operator corresponding to the virial is given by the symmetrized version of its classical counterpart:

$$\hat{G} = \frac{\hat{X}\,\hat{P} + \hat{P}\,\hat{X}}{2}.$$

Note — This symmetrization procedure is necessary whenever the classical quantity we wish to quantize contains products of the type xp, or any product of observables whose quantum-mechanical operators do not commute.

3. The simplest way to see this is to use the general expression for the time evolution of expectation values (Ehrenfest theorem):

$$i\hbar \frac{d}{dt}\langle \hat{A} \rangle = \left\langle \left[\hat{A}, \hat{H}\right] \right\rangle + \left\langle \frac{\partial \hat{A}}{\partial t} \right\rangle .$$

When applied to this case, we have

$$i\hbar \frac{d}{dt}\langle \hat{X}^2 \rangle = \left\langle \left[\hat{X}^2, \hat{H}\right] \right\rangle .$$

and so we must calculate this commutator:

$$\begin{aligned}
\left[\hat{X}^2, \hat{H}\right] &= \frac{1}{2m}\left[\hat{X}^2, \hat{P}^2\right] + \cancelto{0}{\frac{1}{2m}\left[\hat{X}^2, V(\hat{X})\right]} \\
&= \frac{1}{2m}\left(\hat{X}\left[\hat{X}, \hat{P}^2\right] + \left[\hat{X}, \hat{P}^2\right]\hat{X}\right) \\
&= \frac{1}{m}\left(\hat{X} i\hbar \hat{P} + i\hbar \hat{P}\hat{X}\right) \\
&= \frac{2i\hbar}{m}\,\hat{G}
\end{aligned}$$

Therefore, plugging back into the previous expression above we conclude that

$$\frac{d}{dt}\langle \hat{X}^2 \rangle = \frac{2}{m}\,\langle \hat{G} \rangle \qquad \boxdot$$