

Solutions to selected problems

Chapter 1

- 1.1** Yes, because in this case even in the initial state some properties would not be determined and therefore also the properties of future states could not be precisely defined. As a consequence, it would be also impossible to predict future properties.
- 1.2** Not necessarily. In principle, one can imagine the existence of a “discrete” world. However, it would still be necessary to have some laws allowing to infer deterministically a future (or past) state from a given initial (or final) state.
- 1.4** Consider the Jacobi identity (Eq. (1.10d)) and take $h = H$. The first two terms of the rhs are then identically zero and therefore

$$\{H, \{f, g\}\} = 0.$$

- 1.5** $\wp(45^\circ) = 1$, $\wp(135^\circ) = 0$. As a matter of fact, since the component states $|v\rangle$ and $|h\rangle$ are equally weighted in the superposition (1.79), the latter represents the state of a photon with polarization oriented at 45° relative to the horizontal axis. On the contrary, such a state will not pass the filter at 135° as this orientation is orthogonal to the polarization of the state (1.79).
- 1.6** Since $|j\rangle$ and $|k\rangle$ are elements of an orthonormal basis, we have $\langle j | k \rangle$ for $j \neq k$ and 0 1 for $j = k$.
- 1.7** $\hat{P}_k |\psi\rangle = c_k |k\rangle$.
- 1.9** The norm of the vector $|\varphi\rangle = c_k |k\rangle$ is $\|\varphi\| = |c_k|^2$. It is $\|\varphi\| \leq 1$ since $\sum_{j=1}^N |c_j|^2 = 1$, being $\|\varphi\| = 1$ if and only if $c_j = \delta_{jk}$. Physically this means that the projector acts as a filter and therefore it selects a subensemble of the initial ensemble.
- 1.10** Let us assume that $|\xi\rangle$ is in an n -dimensional Hilbert space and expand it as

$$|\xi\rangle = \sum_j c_j |j\rangle,$$

where $|j\rangle$ is an orthonormal basis for this space. It is then easy to show that

$$\begin{pmatrix} c_1^* & c_2^* & \dots & c_n^* \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \dots \\ c_n \end{pmatrix} = 1,$$

since $\sum_{j=1}^n |c_j|^2 = 1$ according to the normalization condition.

- 1.11** We can imagine of having N “boxes” (one for each oscillator) each of them with a certain number of energy quanta $\epsilon(v)$. We are able to calculate w_E , which becomes

the total number of different ways in which we can arrange the n_ϵ quanta among the N oscillators (or boxes), i.e. the total number of permutations of the quanta n_ϵ plus the $N - 1$ partitions¹

$$w_E = \frac{(N - 1 + n_\epsilon)!}{(N - 1)! n_\epsilon!} \simeq \frac{(N + n_\epsilon)^{N + n_\epsilon}}{N^N n_\epsilon^{n_\epsilon}},$$

where in the last equality we have made use of the Stirling formula

$$m! \simeq m^m e^{-m} \sqrt{2\pi m},$$

which is a very good approximation for large m . Consequently, the total entropy is given by

$$S_B^N = k_B N \left[\left(1 + \frac{n_\epsilon}{N}\right) \ln(N + n_\epsilon) - \ln N - \frac{n_\epsilon}{N} \ln n_\epsilon \right].$$

By making use of Eq. (1.62), we obtain the desired result.

1.12 In order to find the solution, let us first compute the differential

$$\begin{aligned} \frac{\partial S_B^N}{\partial U} &= \frac{\partial S_B^N}{\partial N \bar{E}} = \frac{1}{N} \frac{\partial S_B^N}{\partial \bar{E}} \\ &= \frac{k_B}{\epsilon} \left[\ln \left(1 + \frac{\bar{E}}{\epsilon}\right) - \ln \frac{\bar{E}}{\epsilon} \right] \\ &= \frac{k_B}{\epsilon} \ln \frac{\bar{E} + \epsilon}{\bar{E}} = \frac{1}{T}. \end{aligned}$$

From the last equality it follows that

$$\frac{\bar{E} + \epsilon}{\bar{E}} = e^{\epsilon/k_B T},$$

and, finally,

$$\bar{E} = \frac{\epsilon}{e^{\epsilon/k_B T} - 1}.$$

1.13 Applying the Carnot theorem to the upper triangle in Fig. 1.19 we obtain

$$(nv)^2 = \left(\frac{h\nu_s}{c}\right)^2 + \left(\frac{h\nu_i}{c}\right)^2 - 2\frac{h\nu_s}{c} \frac{h\nu_i}{c} \cos \theta.$$

On the other hand energy conservation (Eq. (1.70)) yields

$$mv^2 = 2h(\nu_i - \nu_s).$$

In order to eliminate v , we multiply this last equation times m and equate the resulting rhs to the rhs of the momentum conservation equation and obtain

$$\nu_i - \nu_s = \frac{h}{2mc^2} (\nu_s^2 + \nu_i^2 - 2\nu_s \nu_i \cos \theta).$$

¹ See [Huang 1963, 181–82].

Now, since the wavelength of the scattered photon is only slightly larger than the original one, we have

$$\nu_i \simeq \nu_s \rightarrow \nu_i^2 \simeq \nu_s^2 \simeq \nu_i \nu_s.$$

Consequently,

$$\nu_i - \nu_s = \frac{h}{mc^2} \nu_i \nu_s (1 - \cos \theta).$$

Replacing $\nu_i = \frac{c}{\lambda_i}$ and $\nu_s = \frac{c}{\lambda_s}$ we finally obtain

$$\lambda_s - \lambda_i = \frac{h}{mc} (1 - \cos \theta) = \frac{2h}{mc} \sin^2 \frac{\theta}{2}.$$

Chapter 2

2.1 Take e.g. $\hat{O}' = \hat{I} - \hat{O}$.

2.2

$$\begin{aligned} \begin{pmatrix} \langle h | \psi \rangle \\ \langle v | \psi \rangle \end{pmatrix} &= \begin{bmatrix} \langle h | b \rangle & \langle h | b_{\perp} \rangle \\ \langle v | b \rangle & \langle v | b_{\perp} \rangle \end{bmatrix} \begin{pmatrix} \langle b | \psi \rangle \\ \langle b_{\perp} | \psi \rangle \end{pmatrix} \\ &= \begin{pmatrix} \langle h | b \rangle \langle b | \psi \rangle + \langle h | b_{\perp} \rangle \langle b_{\perp} | \psi \rangle \\ \langle v | b \rangle \langle b | \psi \rangle + \langle v | b_{\perp} \rangle \langle b_{\perp} | \psi \rangle \end{pmatrix} \\ &= \begin{pmatrix} \langle h | \psi \rangle \\ \langle v | \psi \rangle \end{pmatrix}. \end{aligned}$$

The last passage is due to the well-known property of projectors

$$|b\rangle \langle b| + |b_{\perp}\rangle \langle b_{\perp}| = \hat{P}_b + \hat{P}_{b_{\perp}} = \hat{I}.$$

2.3 Let us write the transposed conjugate of \hat{U} :

$$\hat{U}^{\dagger} = \begin{bmatrix} \langle h | b \rangle^* & \langle v | b \rangle^* \\ \langle h | b_{\perp} \rangle^* & \langle v | b_{\perp} \rangle^* \end{bmatrix} = \begin{bmatrix} \langle b | h \rangle & \langle b | v \rangle \\ \langle b_{\perp} | h \rangle & \langle b_{\perp} | v \rangle \end{bmatrix}.$$

Then we have

$$\begin{aligned} \hat{U} \hat{U}^{\dagger} &= \begin{bmatrix} \langle h | b \rangle & \langle h | b_{\perp} \rangle \\ \langle v | b \rangle & \langle v | b_{\perp} \rangle \end{bmatrix} \begin{bmatrix} \langle b | h \rangle & \langle b | v \rangle \\ \langle b_{\perp} | h \rangle & \langle b_{\perp} | v \rangle \end{bmatrix} \\ &= \begin{bmatrix} \langle h | b \rangle \langle b | h \rangle + \langle h | b_{\perp} \rangle \langle b_{\perp} | h \rangle & \langle h | b \rangle \langle b | v \rangle + \langle h | b_{\perp} \rangle \langle b_{\perp} | v \rangle \\ \langle v | b \rangle \langle b | h \rangle + \langle v | b_{\perp} \rangle \langle b_{\perp} | h \rangle & \langle v | b \rangle \langle b | v \rangle + \langle v | b_{\perp} \rangle \langle b_{\perp} | v \rangle \end{bmatrix} \\ &= \begin{bmatrix} \langle h | (|b\rangle \langle b| + |b_{\perp}\rangle \langle b_{\perp}|) | h \rangle & \langle h | (|b\rangle \langle b| + |b_{\perp}\rangle \langle b_{\perp}|) | v \rangle \\ \langle v | (|b\rangle \langle b| + |b_{\perp}\rangle \langle b_{\perp}|) | h \rangle & \langle v | (|b\rangle \langle b| + |b_{\perp}\rangle \langle b_{\perp}|) | v \rangle \end{bmatrix} \\ &= \begin{bmatrix} \langle h | h \rangle & \langle h | v \rangle \\ \langle v | h \rangle & \langle v | v \rangle \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \\ &= \hat{I}, \end{aligned}$$

since $(|b\rangle \langle b| + |b_{\perp}\rangle \langle b_{\perp}|) = \hat{I}$. Similarly it can be shown that $\hat{U}^{\dagger} \hat{U} = \hat{I}$.

2.6 From the condition of unitarity

$$\begin{aligned}
\hat{O} \hat{O}^\dagger &= \begin{bmatrix} a & b \\ c & d \end{bmatrix} \begin{bmatrix} a^* & c^* \\ b^* & d^* \end{bmatrix} \\
&= \begin{bmatrix} |a|^2 + |b|^2 & ac^* + bd^* \\ a^*c + b^*d & |c|^2 + |d|^2 \end{bmatrix} \\
&= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}
\end{aligned}$$

we derive the following relations

$$\begin{aligned}
|a|^2 + |b|^2 &= 1, \\
|c|^2 + |d|^2 &= 1, \\
ac^* + bd^* &= 0.
\end{aligned}$$

Similarly, from the condition of Hermiticity

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix} = \begin{bmatrix} a^* & c^* \\ b^* & d^* \end{bmatrix}$$

we obtain that a and d are real and that $c = b^*$. Collecting these results, we derive that $b(a + d)$ and $a^2 = d^2$. From these relations it follows either that $a = d$, and in this case $b = 0$ and \hat{O} is a multiple of identity, or that $a = -d$, and in this case we have

$$\hat{O} = \begin{bmatrix} a & b \\ b^* & -a \end{bmatrix},$$

2.7 The solution of the problem is

$$\begin{aligned}
\langle b | \hat{O}_P | b \rangle &= (\langle v | c_v^* + \langle h | c_h^*) (|v\rangle \langle v| - |h\rangle \langle h|) (c_v | v\rangle + c_h | h\rangle) \\
&= (\langle v | c_v^* + \langle h | c_h^*) (c_v | v\rangle - c_h | h\rangle) \\
&= |c_v|^2 - |c_h|^2.
\end{aligned}$$

2.8 Let us take a generic ket $|\psi\rangle$. Then,

$$\begin{aligned}
\hat{O} |\psi\rangle &= \sum_j \hat{O} |o_j\rangle \langle o_j | \psi \rangle \\
&= \sum_j o_j |o_j\rangle \langle o_j | \psi \rangle \\
&= \sum_j o_j \hat{P}_j |\psi\rangle,
\end{aligned}$$

where the $|o_j\rangle$ are eigenkets of \hat{O} . Since these equalities must be valid for any $|\psi\rangle$, it follows that $\hat{O} = \sum_j o_j \hat{P}_j$.

2.9 We proceed as follows:

(a) Let us take the usual basis

$$|b_1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |b_2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

We have to find the vectors $|o_1\rangle$ and $|o_2\rangle$ and the (complex) numbers o_1 and o_2 such that

$$\begin{aligned} \hat{O} |o_1\rangle &= o_1 |o_1\rangle, \\ \hat{O} |o_2\rangle &= o_2 |o_2\rangle. \end{aligned}$$

The characteristic polynomial is given by

$$\begin{vmatrix} \lambda & \iota \\ -\iota & \lambda \end{vmatrix} = \lambda^2 - 1,$$

whose zeros (eigenvalues) are $\lambda_{1,2} = \pm 1$. Let us take the eigenvalues $o_1 = +1$ and $o_2 = -1$. Rewriting explicitly the first eigenvalue equation, we must have

$$\begin{bmatrix} 0 & -\iota \\ \iota & 0 \end{bmatrix} \begin{pmatrix} o_1^1 \\ o_1^2 \end{pmatrix} = \begin{pmatrix} o_1^1 \\ o_1^2 \end{pmatrix}$$

that yields $o_1^2 = \iota o_1^1$. The normalized eigenvector $|o_1\rangle$ will then given by

$$|o_1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \iota \end{pmatrix}.$$

With a similar procedure we find

$$|o_2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -\iota \end{pmatrix}.$$

Notice that \hat{O} is Hermitian, $|o_1\rangle$ and $|o_2\rangle$ are orthogonal, i.e. $\langle o_1 | o_2 \rangle = 0$. We have constructed the eigenvectors so that they are also normalized, that is $\langle o_j | o_k \rangle = \delta_{jk}$. In other words, $\{|o_1\rangle, |o_2\rangle\}$ is an orthonormal basis on the bidimensional Hilbert space.

(b) The diagonalizing matrix is simply given by

$$\hat{U} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ \iota & -\iota \end{bmatrix}.$$

Finally, the diagonal form of \hat{O} is

$$\begin{aligned} \hat{O}' &= \hat{U}^\dagger \hat{O} \hat{U} \\ &= \frac{1}{2} \begin{bmatrix} 1 & -\iota \\ 1 & +\iota \end{bmatrix} \begin{bmatrix} 0 & -\iota \\ \iota & 0 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ \iota & -\iota \end{bmatrix} \\ &= \frac{1}{2} \begin{bmatrix} 1 & -\iota \\ 1 & +\iota \end{bmatrix} \begin{bmatrix} 1 & -1 \\ \iota & \iota \end{bmatrix} \\ &= \frac{1}{2} \begin{bmatrix} 2 & 0 \\ 0 & -2 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \end{aligned}$$

2.10 The result is

$$\frac{9}{16}N.$$

2.15 The momentum eigenfunctions in the momentum representation are

$$\begin{aligned}\tilde{\varphi}_{p_0}(p_x) &= \frac{1}{\sqrt{2\pi}} \int dx e^{-\frac{i}{\hbar} p_x x} \varphi_{p_0}(x) \\ &= \frac{1}{\sqrt{2\pi}} \int dx e^{-\frac{i}{\hbar} (p_x - p_0)x} \\ &= \delta(p_x - p_0).\end{aligned}$$

2.16 The position eigenfunctions in the momentum representation are

$$\begin{aligned}\tilde{\varphi}_{x_0}(p_x) &= \frac{1}{\sqrt{2\pi}} \int dx e^{-\frac{i}{\hbar} p_x x} \varphi_{x_0}(x) \\ &= \frac{1}{\sqrt{2\pi}} \int dx e^{-\frac{i}{\hbar} p_x x} \delta(x - x_0) \\ &= \frac{1}{\sqrt{2\pi}} e^{-\frac{i}{\hbar} p_x x_0}.\end{aligned}$$

In the general case we have

$$\tilde{\varphi}_x(p_x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{i}{\hbar} p_x x}.$$

2.17 We proceed as follows:

$$\begin{aligned}\int_{-\infty}^{+\infty} dp_x |\tilde{\psi}(p_x)|^2 &= \int_{-\infty}^{+\infty} dp_x \tilde{\psi}(p_x) \tilde{\psi}^*(p_x) \\ &= \int_{-\infty}^{+\infty} dp_x \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dx \psi(x) e^{-\frac{i}{\hbar} p_x x} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dx' \psi^*(x') e^{\frac{i}{\hbar} p_x x'} \\ &= \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dx' \psi(x) \psi^*(x') \frac{1}{2\pi} \int_{-\infty}^{+\infty} dp_x e^{\frac{i}{\hbar} p_x (x - x')} \\ &= \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dx' \psi(x) \psi^*(x') \delta(x - x') \\ &= \int_{-\infty}^{+\infty} dx |\psi(x)|^2.\end{aligned}$$

2.18 First, calculate

$$\begin{aligned}x\psi(x) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dp_x x \tilde{\psi}(p_x) e^{\frac{i}{\hbar} p_x x} \\ &= \frac{1}{\sqrt{2\pi}} \tilde{\psi}(p_x) \frac{\hbar}{i} e^{\frac{i}{\hbar} p_x x} \Big|_{-\infty}^{+\infty} - \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dp_x \frac{\hbar}{i} e^{\frac{i}{\hbar} p_x x} \frac{\partial \tilde{\psi}(p_x)}{\partial p_x} \\ &= \frac{i\hbar}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dp_x e^{\frac{i}{\hbar} p_x x} \frac{\partial \tilde{\psi}(p_x)}{\partial p_x},\end{aligned}$$

where we have made use of the inverse Fourier transform (2.150a) and of integration by parts. If we substitute this result into the definition of the expectation value of \hat{x} , we obtain

$$\begin{aligned}\langle \hat{x} \rangle &= \int_{-\infty}^{+\infty} dx \psi^*(x) \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dp_x \, i\hbar e^{\frac{i}{\hbar} p_x x} \frac{\partial \tilde{\psi}(p_x)}{\partial p_x} \\ &= \int_{-\infty}^{+\infty} dp_x \left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dx \psi^*(x) e^{\frac{i}{\hbar} p_x x} \right] i\hbar \frac{\partial \tilde{\psi}(p_x)}{\partial p_x} \\ &= \int_{-\infty}^{+\infty} dp_x \tilde{\psi}^*(p_x) i\hbar \frac{\partial \tilde{\psi}(p_x)}{\partial p_x}.\end{aligned}$$

This has to be equal to the expectation value of \hat{x} computed in the momentum representation, i.e.

$$\langle \hat{x} \rangle = \int_{-\infty}^{+\infty} dp_x \tilde{\psi}^*(p_x) \hat{x} \tilde{\psi}(p_x).$$

By comparison, we find

$$\hat{x} \tilde{\psi}(p_x) = i\hbar \frac{\partial \tilde{\psi}(p_x)}{\partial p_x}.$$

2.19 We have

$$\hat{P}(x) |p_x\rangle = |x\rangle \langle x | p_x\rangle = \varphi_p(x) |x\rangle,$$

where $\varphi_p(x) |x\rangle$ is the eigenfunction of the momentum operator corresponding to the eigenvalue p_x , that is

$$\varphi_p(x) = \frac{1}{\sqrt{2\pi}} e^{\frac{i}{\hbar} p_x x}.$$

This shows that the action of the position projector $\hat{P}(x)$ onto the momentum eigenvector $|p_x\rangle$ (in which the position is completely undetermined) selects the position eigenvector $|x\rangle$ with a weight that is given by $\varphi_p(x)$.

2.22 The delta function can be obtained as a limit of a normalized Gaussian

$$f_a(x) = \frac{1}{\sqrt{2\pi}a} e^{-\frac{x^2}{2a^2}},$$

with $a > 0$, that is

$$\delta(x) = \lim_{a \rightarrow 0} f_a(x).$$

Then, we have

$$\begin{aligned}\delta^2(x) &= \lim_{a \rightarrow 0} f_a^2(x) \\ &= \lim_{a \rightarrow 0} \frac{1}{2\pi a^2} e^{-\frac{x^2}{a^2}},\end{aligned}$$

from which we obtain

$$\begin{aligned}\int_{-\infty}^{+\infty} dx \delta^2(x) &= \frac{1}{2\pi} \int_{-\infty}^{+\infty} dx \lim_{a \rightarrow 0} \frac{1}{a^2} e^{-\frac{x^2}{a^2}} \\ &= \frac{1}{2\pi} \lim_{a \rightarrow 0} \frac{1}{a^2} \int_{-\infty}^{+\infty} dx e^{-\frac{x^2}{a^2}} \\ &= \frac{1}{2\sqrt{\pi}} \lim_{a \rightarrow 0} \frac{1}{a} = +\infty.\end{aligned}$$

2.24 $\Delta x \Delta E \geq \frac{1}{2} \frac{\hbar p_0}{m}.$

2.26 The solution is given by

$$\begin{aligned}[\hat{p}_x, f(\hat{x})] &= \frac{\hbar}{i} \frac{\partial}{\partial x} f(\hat{x}) - \frac{\hbar}{i} f(\hat{x}) \frac{\partial}{\partial x} \\ &= \frac{\hbar}{i} f'(\hat{x}) + \frac{\hbar}{i} f(\hat{x}) \frac{\partial}{\partial x} - \frac{\hbar}{i} f(\hat{x}) \frac{\partial}{\partial x} \\ &= \frac{\hbar}{i} f'(\hat{x})\end{aligned}$$

2.30 With $T = 0$ and $R = 1$ we have

$$|f_1\rangle = -\frac{1}{\sqrt{2}} e^{i\phi} (|3\rangle + i|4\rangle),$$

which, up to the irrelevant global phase factor, corresponds to the state $|1\rangle$. With $T = 1$ and $R = 0$, we have

$$|f_0\rangle = \frac{1}{\sqrt{2}} (-|3\rangle + i|4\rangle),$$

which corresponds to the state $|2\rangle$. Finally, with $T = R = 1/\sqrt{2}$, we have

$$\begin{aligned}|f_{1/2}\rangle &= \frac{1}{2} [-(1 + e^{i\phi})|3\rangle + i(1 - e^{i\phi})|4\rangle] \\ &= \frac{1}{\sqrt{2}} \left[\frac{1}{\sqrt{2}} (-|3\rangle + i|4\rangle) - \frac{1}{\sqrt{2}} e^{i\phi} (|3\rangle + i|4\rangle) \right] \\ &= \frac{1}{\sqrt{2}} (|f_0\rangle - e^{i\phi} |f_1\rangle).\end{aligned}$$

2.31 The examination of Sec. 2.4 shows that there are cases in which an event occurs (a certain detector clicks, a state of affairs described by the proposition c) and not withstanding the object system is neither in the state expressed by the proposition a' , nor in the state expressed by the proposition a'' . This means that, in these cases, it is true that

$$[c \wedge (a' \vee a'')] \wedge \neg [(c \wedge a') \vee (c \wedge a'')],$$

from which we easily derive that it is also true that $\neg [(c \wedge a') \vee (c \wedge a'')]$ and, therefore, that

$$\neg (c \wedge a') \quad \text{and} \quad \neg (c \wedge a'')$$

are also true. This means that, in the first case, either c or a' must be false, and, in the second case either c or a'' . However, we have assumed c to be true. Then, both a' and a'' are false. This means that we have a situation in which $a' \vee a''$ is true (by definition) but also both $\neg a'$ and $\neg a''$ are. By substituting a' to $\neg a'$ as well as a'' to $\neg a''$ we obtain that also $\neg(a' \wedge a'')$ is true, which is the desired result.

Chapter 3

3.2 It is straightforward to prove the result given the linearity of the Schrödinger equation.

3.3 $\psi(x) = \frac{1}{\sqrt{2\pi}} e^{\pm i k x}$. These are the plane waves described in Subsecs. 2.2.4 and 2.2.6. They are doubly degenerate: in fact, the plus and minus signs correspond to “waves” moving from left to right and from right to left, respectively, both having the same positive energy $E = \frac{\hbar^2 k^2}{2m}$.

3.4 At time $t_0 = 0$ and t we have

$$\tilde{\psi}(p_x, 0) = \sum_n c_n^{(0)} \tilde{\psi}_n(p_x) \quad \text{and} \quad \tilde{\psi}(p_x, t) = \sum_n e^{-\frac{i}{\hbar} E_n t} c_n^{(0)} \tilde{\psi}_n(p_x)$$

where

$$\tilde{\psi}_n(p_x) = \langle p_x | \psi_n \rangle \quad \text{and} \quad \tilde{\psi}_n(p_x, t) = \langle p_x | \psi(t) \rangle.$$

3.5 Let us rewrite Eq. (3.26) as

$$\psi(x, t) = \sum_n c_n(t) \psi_n(x),$$

from which we obtain

$$\begin{aligned} \int dx |\psi(x, t)|^2 &= \int dx \sum_m c_m^*(t) \psi_m^*(x) \sum_n c_n(t) \psi_n(x) \\ &= \sum_{n,m} c_n(t) c_m^*(t) \int dx \psi_m^*(x) \psi_n(x) \\ &= \sum_n |c_n(t)|^2 = \sum_n \left| e^{-\frac{i}{\hbar} E_n t} c_n(0) \right|^2 \\ &= \sum_n |c_n(0)|^2 = 1. \end{aligned}$$

where

$$\int dx \psi_m^*(x) \psi_n(x) = \delta_{n,m}.$$

3.7 We have

$$\psi(t) = \int dk c(k) e^{i(kx - \omega_k t)}, \quad \text{where} \quad \omega_k = \frac{E}{\hbar} = \hbar \frac{k^2}{2m}.$$

3.10 First let us compute the mean value of the position²

$$\begin{aligned}
 \langle \hat{x} \rangle &= \int_0^a dx \psi_n^*(x) x \psi_n(x) \\
 &= \frac{2}{a} \int_0^a dx x \sin^2 \left(\frac{n\pi}{a} x \right) \\
 &= \frac{2a}{(n\pi)^2} \int_0^{n\pi} dy y \sin^2 y \\
 &= \frac{a}{2},
 \end{aligned}$$

where we have made use of the fact that we are in the position representation and that $\psi_n^*(x) = \psi_n(x)$, as well as the mean value of the square of the position³

$$\begin{aligned}
 \langle \hat{x}^2 \rangle &= \frac{2}{a} \int_0^a dx x^2 \sin^2 \left(\frac{n\pi}{a} x \right) \\
 &= \frac{2a^2}{(n\pi)^3} \int_0^{n\pi} dy y^2 \sin^2 y \\
 &= \frac{a^2}{3} - \frac{1}{2} \left(\frac{a}{n\pi} \right)^2.
 \end{aligned}$$

Analogously, we calculate the mean value of the momentum

$$\begin{aligned}
 \langle \hat{p}_x \rangle &= -i\hbar \frac{2}{a} \int_0^a dx \sin \left(\frac{n\pi}{a} x \right) \frac{\partial}{\partial x} \sin \left(\frac{n\pi}{a} x \right) \\
 &= \frac{2\hbar}{ia} \frac{n\pi}{a} \int_0^a dx \sin \left(\frac{n\pi}{a} x \right) \cos \left(\frac{n\pi}{a} x \right) \\
 &= \frac{h}{2ia} \left[-\frac{1}{2\pi} \cos \left(\frac{2n\pi}{a} x \right) \right]_0^a \\
 &= 0,
 \end{aligned}$$

and of the square of the momentum

$$\begin{aligned}
 \langle \hat{p}_x^2 \rangle &= -\hbar^2 \frac{2}{a} \int_0^a dx \sin \left(\frac{n\pi}{a} x \right) \frac{\partial^2}{\partial x^2} \sin \left(\frac{n\pi}{a} x \right) \\
 &= \frac{2\hbar^2}{a} \frac{n^2\pi^2}{a^2} \int_0^a dx \sin^2 \left(\frac{n\pi}{a} x \right)
 \end{aligned}$$

² See [Gradstein/Ryshik 1981, 3.821].

³ See [Gradstein/Ryshik 1981, 2.631.2].

$$\begin{aligned}
&= \frac{\hbar^2 n}{2a^2 \pi} \left[\frac{1}{2} \left(\frac{n\pi}{a} x \right) - \sin \left(\frac{n\pi}{a} x \right) \cos \left(\frac{n\pi}{a} x \right) \right]_0^{n\pi} \\
&= \frac{\hbar^2 n^2}{4a^2}.
\end{aligned}$$

Then, we calculate the uncertainties of position and momentum

$$\Delta p_x = \frac{nh}{2a}, \quad \Delta x = a \sqrt{\frac{1}{12} - \frac{1}{2n^2 \pi^2}},$$

and finally obtain the uncertainty relation

$$\Delta x \Delta p_x = \frac{\hbar}{2} \left[\sqrt{\frac{n^2 \pi^2}{3} - 2} \right].$$

Since the square root is certainly a growing function of n for $n \geq 1$, in order to verify that the uncertainty relation is always satisfied it is sufficient to prove that, for $n = 1$, it is ≥ 1 . A direct calculation shows that

$$\sqrt{\frac{\pi^2}{3} - 2} = 1.136.$$

3.11 The three-dimensional stationary Schrödinger equation for the wave function in the position representation reads as

$$\left[-\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) + V(x, y, z) \right] \psi(x, y, z) = E \psi(x, y, z).$$

For a particle in a “cubic” box, we have $V(x, y, z) = 0$ inside the box, so that the previous equation becomes

$$-\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \psi(x, y, z) = E \psi(x, y, z).$$

with the boundary conditions

$$\psi(x, y, z) = 0, \quad \text{for } x < 0, x > a; y < 0, y > b; z < 0, z > c.$$

This problem is *separable*, i.e. $\hat{H} = \hat{H}_1(x) + \hat{H}_2(y) + \hat{H}_3(z)$, where

$$\hat{H}_1(x) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2},$$

and similar expressions for $\hat{H}_2(y)$ and $\hat{H}_3(z)$. In

$$\psi(x, y, z) = \psi^{(1)}(x) \cdot \psi^{(2)}(y) \cdot \psi^{(3)}(z),$$

and

$$E = E_x + E_y + E_z.$$

The required solution therefore reduces to

$$\psi_{n_x, n_y, n_z}(x, y, z) = \psi_{n_x}^{(1)}(x) \cdot \psi_{n_y}^{(2)}(y) \cdot \psi_{n_z}^{(3)}(z),$$

with

$$\psi_{n_x}^{(1)}(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n_x \pi}{a} x\right),$$

$$\psi_{n_y}^{(2)}(y) = \sqrt{\frac{2}{b}} \sin\left(\frac{n_y \pi}{b} y\right),$$

$$\psi_{n_z}^{(3)}(z) = \sqrt{\frac{2}{c}} \sin\left(\frac{n_z \pi}{c} z\right),$$

and

$$E_{n_x} = \frac{\pi \hbar^2}{2ma^2} n_x^2,$$

$$E_{n_y} = \frac{\pi \hbar^2}{2mb^2} n_y^2,$$

$$E_{n_z} = \frac{\pi \hbar^2}{2mc^2} n_z^2.$$

3.12 Referring to Fig. 3.8(b), the transformation effected by an asymmetric beam splitter should satisfy the following constraints:

$$\hat{U}_{\text{BS}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \propto \begin{pmatrix} T \\ \iota R \end{pmatrix}$$

$$\hat{U}_{\text{BS}} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \propto \begin{pmatrix} \iota R \\ T \end{pmatrix}.$$

The requirement of unitarity leads us to the final form

$$\hat{U}_{\text{BS}} = \begin{bmatrix} T & \iota R^* \\ \iota R & T^* \end{bmatrix}.$$

3.13 We have

$$\hat{U}_t |\psi\rangle = e^{-\frac{i}{\hbar} \hat{H} t} \sum_j c_j |\psi_j\rangle = \sum_j c_j e^{-\frac{i}{\hbar} E_j t} |\psi_j\rangle,$$

where use has been made of the eigenvalue equation

$$\hat{H} |\psi_j\rangle = E_j |\psi_j\rangle.$$

Now, it is clear that

$$c_j(t) = c_j e^{-\frac{i}{\hbar} E_j t} \neq 0, \quad \text{if } c_j \neq 0.$$

Furthermore, we also have that the probabilities of the energy eigenvalues $\wp_j(t) = |c_j(t)|^2 = \wp_j(0)$ are constant under time evolution.

Note that, in the case of beam-splitting (see Subsec. 3.5.2), the vectors

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad |2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

are neither eigenvectors of the beam-splitter unitary transformation

$$\hat{U}_{\text{BS}} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & i \\ i & 1 \end{bmatrix}.$$

nor of the Hermitian operator \hat{O} that is the generator of the transformation, i.e. $\hat{U}_{\text{BS}} = e^{i\hat{O}}$. This is the reason why certain superposition states of the basis vectors $|1\rangle$ and $|2\rangle$ may be transformed into $|1\rangle$ or $|2\rangle$ under the unitary transformation \hat{U}_{BS} . For instance, the state $\frac{1}{\sqrt{2}}(|1\rangle - i|2\rangle)$ is transformed by \hat{U}_{BS} into $|1\rangle$.

3.14 This result may be proved by taking into account the uniqueness of the unitary transformation $\hat{U}^\dagger = \hat{U}^{-1}$ (its deterministic nature). If this connection had to be not completely clear, see Sec. 15.2.

3.15 We have

$$\hat{H}^{\text{H}}(t) = \hat{U}_t^\dagger \hat{H}^{\text{S}} \hat{U}_t = \hat{U}_t^\dagger \hat{U}_t \hat{H}^{\text{S}} = \hat{H}^{\text{S}},$$

since $\hat{H}^{\text{S}} = \hat{H}$ commutes with $\hat{U}_t = e^{-\frac{i}{\hbar}\hat{H}t}$.

3.17 We have to show that

$$[[\hat{O}, \hat{O}'], \hat{H}] = 0.$$

The explicit calculation is

$$\begin{aligned} [[\hat{O}, \hat{O}'], \hat{H}] &= [\hat{O}\hat{O}', \hat{H}] - [\hat{O}'\hat{O}, \hat{H}] \\ &= \hat{O}\hat{O}'\hat{H} - \hat{H}\hat{O}\hat{O}' - \hat{O}'\hat{O}\hat{H} + \hat{H}\hat{O}'\hat{O} \\ &= \hat{H}\hat{O}\hat{O}' - \hat{H}\hat{O}\hat{O}' - \hat{H}\hat{O}'\hat{O} + \hat{H}\hat{O}'\hat{O} \\ &= 0, \end{aligned}$$

since \hat{H} commutes with both \hat{O} and \hat{O}' .

3.19 We can proceed as follows:

$$\begin{aligned} i\hbar \frac{d}{dt} |\psi(t)\rangle_{\text{I}} &= i\hbar \frac{d}{dt} e^{\frac{i}{\hbar}\hat{H}_0 t} |\psi(t)\rangle_{\text{S}} \\ &= i\hbar \left[\frac{i}{\hbar} \hat{H}_0 e^{\frac{i}{\hbar}\hat{H}_0 t} |\psi(t)\rangle_{\text{S}} + e^{\frac{i}{\hbar}\hat{H}_0 t} \frac{d}{dt} |\psi(t)\rangle_{\text{S}} \right] \\ &= \left[-\hat{H}_0 \hat{U}_{H_0, t}^\dagger + \hat{U}_{H_0, t}^\dagger \hat{H} \right] |\psi(t)\rangle_{\text{S}} \\ &= \left[-\hat{U}_{H_0, t}^\dagger \hat{H}_0 + \hat{U}_{H_0, t}^\dagger \hat{H} \right] \hat{U}_{H_0, t} |\psi(t)\rangle_{\text{I}} \\ &= \hat{U}_{H_0, t}^\dagger \left[-\hat{H}_0 + \hat{H} \right] \hat{U}_{H_0, t} |\psi(t)\rangle_{\text{I}} \\ &= \hat{U}_{H_0, t}^\dagger \hat{H}_1 \hat{U}_{H_0, t} |\psi(t)\rangle_{\text{I}} \\ &= \hat{H}_1^{\text{I}}(t) |\psi(t)\rangle_{\text{I}}. \end{aligned}$$

3.22 Given any two operators \hat{O} and \hat{O}' such that $[\hat{O}, \hat{O}'] = -i\hbar$, it is straightforward to prove that (see Prob. 2.25)

$$[\hat{O}^n, \hat{O}'] = -ni\hbar \hat{O}^{n-1}.$$

Using this result, we may compute the commutator

$$\begin{aligned}
 [e^{i\alpha\hat{t}}, \hat{H}] &= \left[\sum_{j=0}^{\infty} \frac{(i\alpha)^j}{j!} \hat{t}^j, \hat{H} \right] = \sum_{j=0}^{\infty} \frac{(i\alpha)^j}{j!} [\hat{t}^j, \hat{H}] \\
 &= - \sum_{j=1}^{\infty} \frac{(i\alpha)^j}{j!} j i \hbar \hat{t}^{j-1} \\
 &= \alpha \hbar \sum_{j=1}^{\infty} \frac{(i\alpha)^{j-1}}{(j-1)!} \hat{t}^{j-1} \\
 &= \alpha \hbar \sum_{n=0}^{\infty} \frac{(i\alpha)^n}{(n)!} \hat{t}^n \\
 &= \alpha \hbar e^{i\alpha\hat{t}}.
 \end{aligned}$$

Therefore,

$$\hat{H} e^{i\alpha\hat{t}} = e^{i\alpha\hat{t}} \hat{H} - \alpha \hbar e^{i\alpha\hat{t}},$$

which yields the desired result.

Chapter 4

4.1 The energy levels are

$$E(i, j, k) = E_x(i) + E_y(j) + E_z(k) = \frac{\pi \hbar^2}{2m} \left(\frac{i^2}{a^2} + \frac{j^2}{b^2} + \frac{k^2}{c^2} \right),$$

and the wave functions are given by

$$\psi_{i,j,k}(\mathbf{r}) = \psi_i(x)\psi_j(y)\psi_k(z) = \sqrt{\frac{8}{abc}} \sin\left(\frac{i\pi}{a}x\right) \sin\left(\frac{j\pi}{b}y\right) \sin\left(\frac{k\pi}{c}z\right).$$

4.3 (a) The normalization coefficients \mathcal{N}_+ and \mathcal{N}_- may be derived from the continuity of the wave function and its first derivative at $x = 0$, that is,

$$\begin{aligned}
 \psi_{<}(0) &= \psi_{>}(0), \\
 \psi'_{<}(0) &= \psi'_{>}(0),
 \end{aligned}$$

from which we obtain the conditions

$$\begin{aligned}
 \mathcal{N}_+ &= 1 + \mathcal{N}_-, \\
 k_1 \mathcal{N}_+ &= k_2 - k_2 \mathcal{N}_-.
 \end{aligned}$$

A simple calculation yields the desired result

$$\begin{aligned}
 \mathcal{N}_- &= \frac{k_2 - k_1}{k_1 + k_2}, \\
 \mathcal{N}_+ &= \frac{2k_2}{k_1 + k_2}.
 \end{aligned}$$

(b) Equations (4.29), together with the previous result, yield

$$\begin{aligned}\frac{T^2}{R^2} &= \frac{\frac{k_1}{k_2} |\mathcal{N}_+|^2}{|\mathcal{N}_-|^2} = \frac{4k_1k_2}{(k_2 - k_1)^2} \\ &= \frac{4\sqrt{1 - \frac{V_0}{E}}}{2 - \frac{V_0}{E} - 2\sqrt{1 - \frac{V_0}{E}}},\end{aligned}$$

from which we finally obtain that $T^2/R^2 = 16/15$.

It should also be noted that, when $E = V_0$, the ratio T^2/R^2 vanishes, and we have a total reflection of the particle at the potential barrier. However, even in this case (and also for $E < V_0$), there is a non-zero probability of finding the particle in the classically forbidden region. Nevertheless, this probability exponentially vanishes with x .

4.4 (a) For $E > V_0$, the wave function is

$$\begin{aligned}\text{for } x \leq 0, \quad \psi_I(x) &= e^{ik_1x} + Ae^{-imathk_1x}, \\ \text{for } 0 \leq x \leq a, \quad \psi_{II}(x) &= Be^{ik_2x} + B'e^{-ik_2x}, \\ \text{for } x \geq a, \quad \psi_{III}(x) &= Ce^{ik_1x},\end{aligned}$$

where

$$k_1 = \frac{1}{\hbar}\sqrt{2mE}, \quad k_2 = \frac{1}{\hbar}\sqrt{2m(E - V_0)}.$$

The constants A , B , B' , and C may be derived from the conditions

$$\begin{aligned}\psi_I(0) &= \psi_{II}(0), \quad \psi_I'(0) = \psi_{II}'(0), \\ \psi_{II}(a) &= \psi_{III}(a), \quad \psi_{II}'(a) = \psi_{III}'(a),\end{aligned}$$

which yield

$$\begin{aligned}1 + A &= B + B', \\ k_1 - k_1A &= k_2B - k_2B', \\ Be^{ik_2a} + B'e^{-ik_2a} &= Ce^{ik_1a}, \\ k_2Be^{ik_2a} - k_2B'e^{-ik_2a} &= k_1Ce^{ik_1a}.\end{aligned}$$

From these conditions we obtain

$$A = \frac{i \frac{k_2^2 - k_1^2}{k_1k_2} \sin(k_2a)}{2 \cos(k_2a) - i \frac{k_1^2 + k_2^2}{k_1k_2} \sin(k_2a)}.$$

In this case, we have

$$R^2 = |A|^2 \quad \text{and} \quad T^2 = k_1 \frac{|C|^2}{k_1} = |C|^2.$$

From $T^2 + R^2 = 1$, we immediately obtain

$$\begin{aligned} T^2 &= |C|^2 = 1 - |A|^2 \\ &= \frac{4k_1^2 k_2^2}{4k_1^2 k_2^2 + (k_1^2 - k_2^2)^2 \sin^2(k_2 a)}. \end{aligned}$$

- (b) For $E < V_0$, k_2 becomes pure imaginary, which implies that the wave function decreases exponentially in region II. The expression for the transmission coefficient may be obtained from the previous result if one replaces k_2 by $i\kappa_2$, where

$$\kappa_2 = \frac{1}{\hbar} \sqrt{2m(V_0 - E)}.$$

- 4.6** We may use an inductive argument. First, we have to verify that Eq. (4.70) is satisfied for $n = 0$ (see Eq. (4.69)). Then, in order to solve the problem, it suffices to show that, if Eq. (4.70) is assumed to be valid for n , i.e.

$$x_{n,n+1} = \sqrt{\frac{(n+1)\hbar}{2m\omega}},$$

then it is also satisfied for $n+1$. We rewrite Eq. (4.68) for $n+1$

$$x_{n+1,n}^2 \omega_{n,n+1} + x_{n+1,n+2}^2 \omega_{n+2,n+1} = \frac{\hbar}{2m},$$

from which, by using the relations $\omega_{n+2,n+1} = \omega$ and $\omega_{n,n+1} = -\omega$, we can derive

$$x_{n+1,n+2} = \sqrt{\frac{(n+2)\hbar}{2m\omega}},$$

that completes the argument.

- 4.7** There are at least two simple ways to obtain this result, both of which do not involve anything but straightforward calculations. The first method is direct inspection of Eq. (4.60). In fact, if $k = n$, we have that $\omega_{nk} = 0$ and therefore $x_{nk} = 0$. The other method starts from the definition of

$$x_{nn} = \langle \hat{x} \rangle_n = \langle n | \hat{x} | n \rangle = \int_{-\infty}^{+\infty} dx \psi_n^*(x) x \psi_n(x) = \int_{-\infty}^{+\infty} dx \psi_n^2(x) x,$$

where we recall that $\psi_n(x) = \langle x | n \rangle$ is the n -th harmonic oscillator (real) eigenfunction. These eigenfunctions are either odd or even functions of x . As a consequence, the integrand of the last equality in the previous equation is necessarily odd, hence the integral over the whole line is zero.

- 4.8** We have

$$\langle n | \hat{p}_x | n \rangle = \int dx \langle n | x \rangle \langle x | \hat{p}_x | n \rangle = \int dx \psi_n^*(x) \frac{\hbar}{i} \frac{\partial}{\partial x} \psi_n(x).$$

Without loss of generality, we may choose the eigenfunctions to be real. Then,

$$\langle n | \hat{p}_x | n \rangle = \frac{\hbar}{i} \int dx \psi_n(x) \frac{\partial}{\partial x} \psi_n(x).$$

Integrating by parts the previous expression, we arrive at the desired result. The same result may be obtained taking into account the fact that the first derivative of an even (odd) function is odd (even).

4.9 We have

$$\begin{aligned} [\hat{a}, \hat{a}^\dagger] &= \frac{m}{2\hbar\omega} \left(\omega^2 [\hat{x}, \hat{x}] + i\omega [\hat{x}, \hat{x}] - i\omega [\hat{x}, \hat{x}] + [\hat{x}, \hat{x}] \right) \\ &= -\frac{im}{\hbar} [\hat{x}, \hat{x}] \\ &= -\frac{i}{\hbar} [\hat{x}, \hat{p}_x] = \hat{I}, \end{aligned}$$

where we have made use of the fact that $[\hat{O}, \hat{O}] = 0$, that $[\hat{O}, \hat{O}'] = -[\hat{O}', \hat{O}]$ (see Eqs. (2.94) and (2.97)), and that $[\hat{x}, \hat{p}_x] = i\hbar$.

4.10 Starting from Eqs. (4.73), we can write the product

$$\begin{aligned} \hat{a}\hat{a}^\dagger &= \frac{m}{2\hbar\omega} (\omega\hat{x} + i\hat{p}_x) (\omega\hat{x} - i\hat{p}_x) \\ &= \frac{1}{2\hbar} \left(m\omega\hat{x}^2 + \frac{\hat{p}_x^2}{m\omega} + i[\hat{p}_x, \hat{x}] \right) \\ &= \frac{1}{\hbar\omega} \left(\frac{1}{2}m\omega^2\hat{x}^2 + \frac{\hat{p}_x^2}{2m} \right) + \frac{1}{2}, \end{aligned}$$

where we have made use of the fact that

$$\hat{x} = \frac{\hat{p}_x}{m} \quad \text{and} \quad [\hat{p}_x, \hat{x}] = -i\hbar.$$

From the above expression and the commutator (Eq. (4.74)) we can derive

$$\hat{H} = \hbar\omega \left(\hat{a}\hat{a}^\dagger - \frac{1}{2} \right) \quad \text{and} \quad \hat{H} = \frac{\hbar\omega}{2} (\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a}).$$

4.11 We have

$$\begin{aligned} [\hat{a}, \hat{N}] &= [\hat{a}, \hat{a}^\dagger\hat{a}] = \hat{a}\hat{a}^\dagger\hat{a} - \hat{a}^\dagger\hat{a}\hat{a} \\ &= [\hat{a}, \hat{a}^\dagger]\hat{a} = \hat{a}, \end{aligned}$$

and

$$\begin{aligned} [\hat{a}^\dagger, \hat{N}] &= [\hat{a}^\dagger, \hat{a}^\dagger\hat{a}] = \hat{a}^\dagger\hat{a}^\dagger\hat{a} - \hat{a}^\dagger\hat{a}\hat{a}^\dagger \\ &= \hat{a}^\dagger[\hat{a}^\dagger, \hat{a}] = -\hat{a}^\dagger. \end{aligned}$$

4.12 We have

$$\begin{aligned} [\hat{a}, (\hat{a}^\dagger)^2] &= \hat{a}\hat{a}^\dagger\hat{a}^\dagger - \hat{a}^\dagger\hat{a}^\dagger\hat{a} \\ &= \hat{a}\hat{a}^\dagger\hat{a}^\dagger - \hat{a}^\dagger\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a}^\dagger\hat{a} \\ &= [\hat{a}, \hat{a}^\dagger]\hat{a}^\dagger + \hat{a}^\dagger[\hat{a}, \hat{a}^\dagger] = 2\hat{a}^\dagger, \end{aligned}$$

and

$$\begin{aligned} [\hat{a}^2, \hat{a}^\dagger] &= \hat{a}\hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a}\hat{a} \\ &= \hat{a}\hat{a}\hat{a}^\dagger - \hat{a}\hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger\hat{a} - \hat{a}^\dagger\hat{a}\hat{a} \\ &= \hat{a}[\hat{a}, \hat{a}^\dagger] + [\hat{a}, \hat{a}^\dagger]\hat{a} = 2\hat{a}, \end{aligned}$$

which can be both generalized by induction. We prove only the first one. Assuming that the relation

$$[\hat{a}, (\hat{a}^\dagger)^n] = n(\hat{a}^\dagger)^{n-1}$$

holds for a given n , we have to prove that it also holds for $n + 1$, that is

$$\begin{aligned} [\hat{a}, (\hat{a}^\dagger)^{n+1}] &= \hat{a}(\hat{a}^\dagger)^n\hat{a}^\dagger - (\hat{a}^\dagger)^n\hat{a}^\dagger\hat{a} \\ &= \hat{a}(\hat{a}^\dagger)^n\hat{a}^\dagger - (\hat{a}^\dagger)^n\hat{a}\hat{a}^\dagger + (\hat{a}^\dagger)^n\hat{a}\hat{a}^\dagger - (\hat{a}^\dagger)^n\hat{a}^\dagger\hat{a} \\ &= [\hat{a}, (\hat{a}^\dagger)^n]\hat{a}^\dagger + (\hat{a}^\dagger)^n[\hat{a}, \hat{a}^\dagger] \\ &= n(\hat{a}^\dagger)^n + (\hat{a}^\dagger)^n = (n+1)(\hat{a}^\dagger)^n. \end{aligned}$$

4.13 Again, we prove this relation by induction. From the second of Eqs. (4.85) we immediately obtain

$$|1\rangle = \hat{a}^\dagger |0\rangle.$$

Assuming that the relation holds for a given n , we must prove that it holds for $n + 1$ as well, that is,

$$|n+1\rangle = \frac{(\hat{a}^\dagger)^{n+1}}{\sqrt{(n+1)!}} |0\rangle.$$

In fact, we have

$$\begin{aligned} \frac{(\hat{a}^\dagger)^{n+1}}{\sqrt{(n+1)!}} |0\rangle &= \frac{\hat{a}^\dagger}{\sqrt{n+1}} \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}} |0\rangle \\ &= \frac{\hat{a}^\dagger}{\sqrt{n+1}} |n\rangle = |n+1\rangle. \end{aligned}$$

4.14 We must have

$$1 = |\mathcal{N}|^2 \int_{-\infty}^{+\infty} dx e^{-\frac{m\omega}{\hbar} x^2}.$$

Using the formula⁴

$$\int_{-\infty}^{+\infty} dy e^{-ay^2} = \sqrt{\frac{\pi}{a}},$$

⁴ See [Gradstein/Ryshik 1981, 3.325].

with $\sqrt{m\omega/\hbar} = a$, we obtain, taking N real for simplicity and without loss of generality (see Property (iv) of Subsec. 3.2.2),

$$\mathcal{N} = \left(\frac{m\omega}{\pi\hbar} \right)^{\frac{1}{4}}.$$

4.16 (i) The first six Hermite polynomials are

$$\begin{aligned} H_0(\zeta) &= 1, & H_1(\zeta) &= 2\zeta, \\ H_2(\zeta) &= 4\zeta^2 - 2, & H_3(\zeta) &= 8\zeta^3 - 12\zeta, \\ H_4(\zeta) &= 16\zeta^4 - 48\zeta^2 + 12, & H_5(\zeta) &= 32\zeta^5 - 160\zeta^3 + 120\zeta. \end{aligned}$$

(iii) We limit ourselves to derive the third recursion relation. Let us start from direct differentiation of the n -th order Hermite polynomial, that is

$$\begin{aligned} \frac{d}{d\zeta} H_n(\zeta) &= (-1)^n 2\zeta e^{\zeta^2} \frac{d^n}{d\zeta^n} e^{-\zeta^2} + (-1)^n e^{\zeta^2} \frac{d^{n+1}}{d\zeta^{n+1}} e^{-\zeta^2} \\ &= 2\zeta (-1)^n e^{\zeta^2} \frac{d^n}{d\zeta^n} e^{-\zeta^2} - (-1)^{n+1} e^{\zeta^2} \frac{d^{n+1}}{d\zeta^{n+1}} e^{-\zeta^2} \\ &= 2\zeta H_n(\zeta) - H_{n+1}(\zeta). \end{aligned}$$

(iv) We start from

$$\frac{d^2}{d\zeta^2} H_n(\zeta) = 2n \frac{d}{d\zeta} H_{n-1}(\zeta) = 4n(n-1) H_{n-2}(\zeta),$$

where we have made use of the first recursion relation in (iii) twice. Replacing the first and the second derivatives into the differential equation as above, we obtain an identity.

4.17 We write the Schrödinger equation as

$$\frac{d^2}{dx^2} \psi(x) + \frac{2m}{\hbar^2} \left(E - \frac{1}{2} m\omega^2 x^2 \right) \psi(x) = 0,$$

and make the change of variable $\xi = x\sqrt{\frac{m\omega}{\hbar}}$. The resulting equation is

$$\frac{d^2}{d\xi^2} \psi(\xi) + \left(\frac{2E}{\hbar\omega} - \xi^2 \right) \psi(\xi) = 0.$$

It is now convenient to consider the asymptotic behavior of $\psi(\xi)$: for large $|\xi|^2$, we may neglect $2E/\hbar\omega$ with respect to ξ^2 and the asymptotic solutions of

$$\frac{d^2}{d\xi^2} \psi(\xi) = \xi^2 \psi$$

are $\psi(\xi) = e^{\pm\xi^2/2}$. Due to the finiteness condition of $\psi(\xi)$ for $\xi \rightarrow \pm\infty$, we have to discard the solution $\psi(\xi) = e^{\xi^2/2}$. As a consequence, it is natural to make the ansatz

$$\psi(\xi) = e^{-\xi^2/2} \varphi(\xi),$$

and obtain for $\varphi(\xi)$ the differential equation

$$\left[\frac{d^2}{d\xi^2} - 2\xi \frac{d}{d\xi} + \left(\frac{2E}{\hbar\omega} - 1 \right) \right] \varphi(\xi) = 0.$$

The solutions of the previous equation with the condition that $\varphi(\xi)$ be finite for finite values of ξ and that it grow at most as a power of ξ for $\xi \rightarrow \pm\infty$ exist only for integer values of $n = E/\hbar\omega - 1/2 \geq 0$ and are given by the Hermite polynomials (see Prob. 4.16) up to a normalization factor. This gives the eigenvalues (Eq. (4.72)) and eigenfunctions (Eq. (4.97)), and represents an alternative solution of the harmonic oscillator problem.⁵

- 4.19** It is always interesting to make a comparison between the quantum results and the corresponding classical ones. In the case of the harmonic oscillator, this is enlightning and relatively straightforward. As we shall see later (in Chs. 9 and 10), however, in general the classical limit in quantum mechanics is far from being obvious. The equation of motion for a one-dimensional classical harmonic oscillator⁶ is

$$x_{\text{cl}}(t) = A \sin(\omega t + \phi),$$

from which

$$\dot{x}_{\text{cl}}(t) = A\omega \cos(\omega t + \phi).$$

The total energy of the system is then given by

$$E_{\text{cl}} = \frac{1}{2}m \left(\dot{x}_{\text{cl}}^2 + \omega^2 x_{\text{cl}}^2 \right) = \frac{1}{2}m\omega^2 A^2,$$

that yields $A = \sqrt{2E_{\text{cl}}/(m\omega^2)}$. In order to obtain the classical mean values, instead of averaging – as in the quantum-mechanical case – over the ensemble, we have to average over a time period of the motion ($\tau = 2\pi/\omega$). We have

$$\overline{x}_{\text{cl}} = 0, \quad \overline{\dot{x}_{\text{cl}}} = 0,$$

whereas

$$\begin{aligned} \overline{x_{\text{cl}}^2} &= \frac{A^2}{\tau} \int_0^\tau dt \sin^2(\omega t + \phi) \\ &= \frac{A^2}{\tau} \int_0^\tau dt \frac{1 - \cos[2(\omega t + \phi)]}{2} = \frac{A^2}{2} = \frac{E_{\text{cl}}}{m\omega^2}, \end{aligned}$$

and

$$\overline{(p_x^2)_{\text{cl}}} = m^2 \overline{\dot{x}_{\text{cl}}^2} = \frac{1}{2}A^2\omega^2 m^2 = mE_{\text{cl}}.$$

⁵ See [Landau/Lifshitz 1976b, Ch. 3].

⁶ See [Goldstein 1950, Chs. 8–9].

Next, we calculate the corresponding quantum-mechanical mean values. We have (see Probs. 4.7 and 4.8)

$$\langle \hat{x} \rangle_{\psi_n} = \langle \hat{p}_x \rangle_{\psi_n} = 0,$$

and

$$\begin{aligned} \langle \hat{x}^2 \rangle_{\psi_n} &= \langle n | \hat{x}^2 | n \rangle = \sum_k \langle n | \hat{x} | k \rangle \langle k | \hat{x} | n \rangle \\ &= \langle n | \hat{x} | n+1 \rangle \langle n+1 | \hat{x} | n \rangle + \langle n | \hat{x} | n-1 \rangle \langle n-1 | \hat{x} | n \rangle \\ &= \frac{\hbar(n+1)}{2m\omega} + \frac{\hbar n}{2m\omega} = \frac{E_n}{m\omega^2}, \end{aligned}$$

where we have made use of Eq. (4.70). Similarly,

$$\begin{aligned} \langle \hat{p}_x^2 \rangle_{\psi_n} &= \langle n | \hat{p}_x^2 | n \rangle = m^2 \langle n | \hat{x}^2 | n \rangle \\ &= m^2 \sum_k \langle n | \hat{x} | k \rangle \langle k | \hat{x} | n \rangle \\ &= m^2 \sum_k i\omega_{nk} x_{nk} i\omega_{kn} x_{kn} \\ &= \frac{1}{2} m\omega\hbar (n+1) + \frac{1}{2} m\omega\hbar n = mE_n. \end{aligned}$$

The results above show a complete correspondence between the classical and the quantum expectation values. This result is valid in this particular case but, due to the Ehrenfest theorem (see Sec. 3.7), it cannot be generalized.

4.20 Using the results of the Prob. 4.19 and Eqs. (2.184), we immediately have

$$\Delta_{\psi_n} x \cdot \Delta_{\psi_n} p_x = \frac{E_n}{\omega} = \hbar \left(n + \frac{1}{2} \right).$$

Here, it is clear that the harmonic oscillator is an exceptional case: the Gaussian wave function of the ground state saturates the uncertainty relation ($\Delta_{\psi_n} x \cdot \Delta_{\psi_n} p_x = \hbar/2$), as happens for all coherent states (the subject of Subsec. 13.4.2). This ensures that the lower bound of the uncertainty product given by Heisenberg relation is the best constraint attainable.

4.21 Under the harmonic-oscillator Hamiltonian

$$\hat{H} = \hbar\omega \left(\hat{N} + \frac{1}{2} \right),$$

any initial state

$$| \psi(0) \rangle = \sum_n c_n | n \rangle$$

evolves according to

$$| \psi(t) \rangle = e^{-\frac{i}{\hbar} \hat{H} t} | \psi(0) \rangle.$$

After one period $\tau = 2\pi/\omega$, we have

$$\begin{aligned} |\psi(\tau)\rangle &= e^{-\frac{i}{\hbar}\hat{H}\tau} |\psi(0)\rangle \\ &= \sum_n c_n e^{-i\omega(\hat{N}+\frac{1}{2})\tau} |n\rangle \\ &= \sum_n c_n e^{-i(n+\frac{1}{2})2\pi} |n\rangle \\ &= e^{-i\pi} |\psi(0)\rangle. \end{aligned}$$

4.22 Let us explicitly derive the x -component of Eq. (4.127). Then, we have

$$\frac{\partial L}{\partial \dot{x}} = mv_x + \frac{e}{c} A_x,$$

with $v_x = \dot{x}$, while we have

$$\frac{\partial L}{\partial x} = -e \frac{\partial U}{\partial x} + \frac{e}{c} \left(v_x \frac{\partial A_x}{\partial x} + v_y \frac{\partial A_y}{\partial x} + v_z \frac{\partial A_z}{\partial x} \right),$$

from which we derive (Eq. (1.15))

$$m \frac{d}{dt} v_x + \frac{e}{c} \frac{d}{dt} A_x = -e \frac{\partial U}{\partial x} + \frac{e}{c} \left(v_x \frac{\partial A_x}{\partial x} + v_y \frac{\partial A_y}{\partial x} + v_z \frac{\partial A_z}{\partial x} \right).$$

But, making use of Eq. (4.139), we have

$$\frac{dA_x}{dt} = \frac{\partial A_x}{\partial t} + \left(v_x \frac{\partial A_x}{\partial x} + v_y \frac{\partial A_x}{\partial y} + v_z \frac{\partial A_x}{\partial z} \right).$$

Collecting these results together, we obtain

$$\begin{aligned} m \frac{d}{dt} v_x &= e \left[-\frac{\partial A_x}{\partial t} - \frac{\partial U}{\partial x} + v_x \frac{\partial A_x}{\partial x} - v_x \frac{\partial A_x}{\partial x} \right. \\ &\quad \left. - v_y \frac{\partial A_x}{\partial y} - v_z \frac{\partial A_x}{\partial z} + v_y \frac{\partial A_y}{\partial x} + v_z \frac{\partial A_z}{\partial x} \right] \\ &= e \left[-\frac{\partial A_x}{\partial t} - \frac{\partial U}{\partial x} - v_y \left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y} \right) + v_z \left(\frac{\partial A_z}{\partial x} - \frac{\partial A_x}{\partial z} \right) \right]. \end{aligned}$$

Notice that this result corresponds to the x -component of Eq. (4.127), i.e.

$$\frac{d}{dt} p_x = e \left(-\frac{\partial}{\partial x} U - \frac{\partial}{\partial t} A_x \right) + \frac{e}{c} (\mathbf{v} \times \mathbf{B})_x,$$

since the explicit expression for $\mathbf{v} \times \mathbf{B}$ is given by

$$\begin{aligned} \mathbf{v} \times \mathbf{B} &= \mathbf{v} \times (\nabla \times \mathbf{A}) \\ &= \left[v_y \left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y} \right) - v_z \left(\frac{\partial A_x}{\partial z} - \frac{\partial A_z}{\partial x} \right) \right] \mathbf{i} \\ &\quad + \left[v_z \left(\frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z} \right) - v_x \left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y} \right) \right] \mathbf{j} \\ &\quad + \left[v_x \left(\frac{\partial A_x}{\partial z} - \frac{\partial A_z}{\partial x} \right) - v_y \left(\frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z} \right) \right] \mathbf{k}. \end{aligned}$$

One may proceed in a similar way to derive the expressions for the y and z components.

Chapter 5

5.2 Equation (2.117) states that

$$\int dx \varphi_{\xi'}(x) \varphi_{\xi}^*(x) = \delta(\xi - \xi'),$$

where $\varphi_{\xi}(x) = \langle x | \xi \rangle$. It follows that, for $\xi' = \xi$ and $\hat{\rho} = |\xi\rangle \langle \xi|$, we have

$$\text{Tr}(\hat{\rho}) = \int dx \langle x | \hat{\rho} | x \rangle = \infty.$$

5.5 It confirms that there is no unitary transformation from a pure density matrix to a mixtures, since unitary transformations preserve scalar products (and therefore probabilities). This is a further formulation of the measurement problem.

5.6 Let us first compute the density matrix

$$\hat{\rho} = |\psi\rangle \langle \psi| = \frac{1}{2} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}.$$

Its characteristic equation, $\text{Det}(\hat{\rho} - \lambda \hat{I}) = 0$, is

$$\left(\frac{1}{2} - \lambda\right)^2 - \frac{1}{4} = 0,$$

from which we easily obtain the solutions

$$\lambda_1 = 1, \quad \lambda_2 = 0.$$

We can now compute the eigenvectors, which are

$$\begin{aligned} |+\rangle &= \frac{1}{\sqrt{2}} (|h\rangle + |v\rangle), \\ |-\rangle &= \frac{1}{\sqrt{2}} (|h\rangle - |v\rangle). \end{aligned}$$

The diagonalized form of $\hat{\rho}$ is then:

$$\hat{U}^{-1} \hat{\rho} \hat{U} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix},$$

where

$$\hat{U} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}.$$

If we indicate with \hat{P}_1 the diagonalized form of $\hat{\rho}$, it is easy to show that $\hat{\rho}'$ has the form

$$\hat{\rho}' = \frac{1}{2} \hat{P}_1 + \frac{1}{2} \hat{P}_2,$$

where \hat{P}_2 is the projector complementary to \hat{P}_1 .

5.7 It is possible to write $|\Psi\rangle_{12} = |\psi\rangle_1 \otimes |\varphi\rangle_2$, with

$$|\psi\rangle_1 = \frac{1}{\sqrt{2}}(|h\rangle_1 + |v\rangle_1) \quad \text{and} \quad \frac{1}{\sqrt{2}}|\varphi\rangle_2 = (|h\rangle_2 + |v\rangle_2).$$

5.8 It is easy to verify that, if the entangled state $|\Psi\rangle_{12}$ could be written as a product state of $|\psi\rangle_1$ and $|\varphi\rangle_2$, we should have

$$c_{hv} = c_h c'_v \quad \text{and} \quad c_{vh} = c_v c'_h.$$

Now, in order to obtain the entangled state $|\Psi\rangle_{12}$, we must also have $c_h c'_h = c_v c'_v = 0$. However, this would imply that either c_h or c'_h and either c_v or c'_v be equal to zero, which contradicts the fact that neither c_{hv} nor c_{vh} can be zero.

5.9 The state $|\Psi\rangle_{12}$ can be rewritten as (see Prob. 5.7)

$$|\Psi\rangle_{12} = \frac{1}{\sqrt{2}}(|h\rangle_1 + |v\rangle_1) \otimes \frac{1}{\sqrt{2}}(|h\rangle_2 + |v\rangle_2).$$

The reduced density matrices are therefore given by

$$\begin{aligned} \hat{\rho}_1 &= \frac{1}{2}(|h\rangle_1 + |v\rangle_1)(\langle h|_1 + \langle v|_1), \\ \hat{\rho}_2 &= \frac{1}{2}(|h\rangle_2 + |v\rangle_2)(\langle h|_2 + \langle v|_2), \end{aligned}$$

which both describe pure states.

5.10 Let us write the factorized state as

$$\hat{\rho}_{12} = |\psi\rangle_1 \langle\psi| \otimes |\varphi\rangle_2 \langle\varphi|.$$

The first reduced density matrix is

$$\begin{aligned} \hat{\rho}_1 &= |\psi\rangle_1 \langle\psi| \otimes \sum_j {}_2\langle j| \varphi\rangle_2 \langle\varphi| j\rangle_2 \\ &= |\psi\rangle_1 \langle\psi| \otimes \sum_j \left| {}_2\langle j| \varphi\rangle_2 \right|^2 \\ &= |\psi\rangle_1 \langle\psi| \otimes \sum_j |c_j|^2 = |\psi\rangle_1 \langle\psi|, \end{aligned}$$

if $|\varphi\rangle_2$ is normalized and where $\{|j\rangle\}$ is an arbitrary basis in the Hilbert space of the system.

5.11 The reduced density matrix is

$$\hat{\rho}_2 = \begin{bmatrix} |c_{00}|^2 + |c_{10}|^2 & c_{00}c_{01}^* + c_{10}c_{11}^* \\ c_{00}^*c_{01} + c_{10}^*c_{11} & |c_{01}|^2 + |c_{11}|^2 \end{bmatrix}.$$

It is given again by the sum of the diagonal elements of the matrix (5.45) when one interchanges the second and third row and the second and the third column.

5.12 The matrix \hat{C} is given by

$$\hat{C} = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix},$$

and it is clear that $\hat{C} = \hat{C}^\dagger$. Let us now compute

$$\hat{C}\hat{C}^\dagger = \hat{C}^\dagger\hat{C} = \frac{1}{2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix},$$

which is a multiple of the identity operator. Its eigenvalues are degenerate and both $1/2$. Since these are c_n^2 , we have that $c_n = \pm 1/\sqrt{2}$. Moreover, we are free to choose the eigenvectors of $\hat{C}\hat{C}^\dagger$ and $\hat{C}^\dagger\hat{C}$, since any vector is eigenvector of the identity. In particular, we choose

$$\begin{aligned} |v_\alpha\rangle &= |w_\alpha\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle), \\ |v_\beta\rangle &= |w_\beta\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle). \end{aligned}$$

Therefore, we can write

$$\begin{aligned} |\Psi\rangle &= \sum_{n=\alpha}^{\beta} c_n |v_n\rangle |w_n\rangle \\ &= \frac{1}{\sqrt{2}}(|\alpha\rangle |\alpha\rangle - |\beta\rangle |\beta\rangle), \end{aligned}$$

with

$$\begin{aligned} |\alpha\rangle |\alpha\rangle &= \frac{1}{2}(|0\rangle |0\rangle + |1\rangle |1\rangle + |0\rangle |1\rangle + |1\rangle |0\rangle), \\ |\beta\rangle |\beta\rangle &= \frac{1}{2}(|0\rangle |0\rangle + |1\rangle |1\rangle - |0\rangle |1\rangle - |1\rangle |0\rangle). \end{aligned}$$

It is easy to verify that from the two previous equations one obtains again

$$|\Psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle |1\rangle + |1\rangle |0\rangle),$$

as expected. From our calculations, the two unitary matrices are easily derived (they are the matrices whose column vectors are the two vectors $|v_n\rangle$ and $|w_n\rangle$), that is

$$\hat{U} = \hat{U}' = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}.$$

It is finally straightforward to verify that, given these matrices, Eq. (5.51) holds.

- 5.14** The fact that the density operator corresponding to the center of a $(n+1)$ -dimensional (hyper-)sphere is always given by $\frac{1}{n}\hat{I}$, where n is the number of dimensions of the system, can be easily understood by considering that the trace of a density matrix is always equal to 1 (see Property (1.41a)), and the fact that any density matrix may be written as $\hat{\rho} = \sum_{j=1}^n w_j \hat{P}_j$, where again, if $\hat{\rho}$ is a mixture, n are the dimensions of the system.

Chapter 6

6.2 Writing $\hat{\mathbf{L}}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$, we have $[\hat{L}_x, \hat{\mathbf{L}}^2] = [\hat{L}_x, \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2]$, since $[\hat{L}_x, \hat{L}_x^2] = 0$. Moreover,

$$\begin{aligned} [\hat{L}_x, \hat{L}_y^2] &= \hat{L}_x \hat{L}_y^2 - \hat{L}_y^2 \hat{L}_x \\ &= \hat{L}_x \hat{L}_y \hat{L}_y - \hat{L}_y \hat{L}_x \hat{L}_y + \hat{L}_y \hat{L}_x \hat{L}_y - \hat{L}_y \hat{L}_y \hat{L}_x \\ &= [\hat{L}_x, \hat{L}_y] \hat{L}_y + \hat{L}_y [\hat{L}_x, \hat{L}_y] \\ &= i\hbar (\hat{L}_z \hat{L}_y + \hat{L}_y \hat{L}_z) = i\hbar [\hat{L}_z, \hat{L}_y]_+ . \end{aligned}$$

On the other hand, proceeding in an analogous way, we have

$$[\hat{L}_x, \hat{L}_z^2] = -i\hbar (\hat{L}_y \hat{L}_z + \hat{L}_z \hat{L}_y) = i\hbar [\hat{L}_y, \hat{L}_z]_+ .$$

In conclusion $[\hat{L}_x, \hat{\mathbf{L}}^2] = 0$. It is easy to verify that this result holds true also for \hat{L}_y and \hat{L}_z , which proves the desired result.

6.4 Making use of Properties (2.97) and (2.99), and of Eq. (2.174), we obtain

$$\begin{aligned} [\hat{L}_z, \hat{x}] &= [\hat{x} \hat{p}_y - \hat{y} \hat{p}_x, \hat{x}] \\ &= [\hat{x} \hat{p}_y, \hat{x}] - [\hat{y} \hat{p}_x, \hat{x}] \\ &= [\hat{x}, \hat{x}] \hat{p}_y + \hat{x} [\hat{p}_y, \hat{x}] - [\hat{y}, \hat{x}] \hat{p}_x - \hat{y} [\hat{p}_x, \hat{x}] \\ &= i\hbar \hat{y}, \end{aligned}$$

and, similarly,

$$\begin{aligned} [\hat{L}_z, \hat{p}_x] &= [\hat{x} \hat{p}_y, \hat{p}_x] - [\hat{y} \hat{p}_x, \hat{p}_x] \\ &= [\hat{x}, \hat{p}_x] \hat{p}_y + \hat{x} [\hat{p}_y, \hat{p}_x] - [\hat{y}, \hat{p}_x] \hat{p}_x - \hat{y} [\hat{p}_x, \hat{p}_x] \\ &= i\hbar \hat{p}_y. \end{aligned}$$

6.6 For any state vector $|\psi\rangle$ we have (see also Eq. (4.63))

$$\langle \psi | \hat{L}_x^2 | \psi \rangle = \left(\langle \psi | \hat{L}_x^\dagger \right) \left(\hat{L}_x | \psi \rangle \right) \geq 0.$$

Along the same lines, we also have $\langle \psi | \hat{L}_y^2 | \psi \rangle \geq 0$ which, together with the previous equation, proves the result.

6.7 Making use of Eqs. (6.6) and (6.7), it is straightforward to obtain

$$\begin{aligned} [\hat{L}_z, \hat{L}_\pm] &= [\hat{L}_z, \hat{L}_x \pm i\hat{L}_y] = [\hat{L}_z, \hat{L}_x] \pm i[\hat{L}_z, \hat{L}_y] = i\hat{L}_y \pm \hat{L}_x = \pm \hat{L}_\pm, \\ [\hat{L}_+, \hat{L}_-] &= [\hat{L}_x + i\hat{L}_y, \hat{L}_x - i\hat{L}_y] = -i[\hat{L}_x, \hat{L}_y] + i[\hat{L}_y, \hat{L}_x] = 2\hat{L}_z, \\ [\hat{\mathbf{L}}^2, \hat{L}_\pm] &= [\hat{\mathbf{L}}^2, \hat{L}_x \pm i\hat{L}_y] = [\hat{\mathbf{L}}^2, \hat{L}_x] \pm i[\hat{\mathbf{L}}^2, \hat{L}_y] = 0. \end{aligned}$$

6.9 Starting from Eq. (6.30), we apply \hat{L}_- to both sides. Since $\hat{L}_- |l, l\rangle = k |l, l-1\rangle$, we have

$$\hat{L}_- \hat{\mathbf{L}}^2 |l, l\rangle = l(l+1)k |l, l-1\rangle .$$

Given that \hat{L}_- and \hat{I}^2 commute (see Eq. (6.24)), we finally obtain

$$\hat{I}^2 k |l, l-1\rangle = l(l+1)k |l, l-1\rangle,$$

which proves the desired result. Successively applying the lowering operator \hat{L}_- as above, we obtain Eq. (6.31) for any m_l .

6.10 In the case of \hat{L}_z , we have

$$\begin{aligned}\hat{L}_z |1, 1\rangle &= |1, 1\rangle, \\ \hat{L}_z |1, 0\rangle &= 0, \\ \hat{L}_z |1, -1\rangle &= -|1, -1\rangle,\end{aligned}$$

from which the first matrix follows. For \hat{L}_+ , we have

$$\begin{aligned}\hat{L}_+ |1, 1\rangle &= 0, \\ \hat{L}_+ |1, 0\rangle &= \sqrt{2} |1, 1\rangle, \\ \hat{L}_+ |1, -1\rangle &= \sqrt{2} |1, 0\rangle,\end{aligned}$$

from which the second matrix follows. Finally, for \hat{L}_- we have

$$\begin{aligned}\hat{L}_- |1, 1\rangle &= \sqrt{2} |1, 0\rangle, \\ \hat{L}_- |1, 0\rangle &= \sqrt{2} |1, -1\rangle, \\ \hat{L}_- |1, -1\rangle &= 0,\end{aligned}$$

from which the third matrix follows.

6.11 Making use of Eqs. (6.32)–(6.33), we have

$$\frac{\partial(r, \phi, \theta)}{\partial(x, y, z)} = \begin{bmatrix} \cos \phi \sin \theta & \sin \phi \sin \theta & \cos \theta \\ -\frac{1}{r} \frac{\sin \phi}{\sin \theta} & \frac{1}{r} \frac{\cos \phi}{\sin \theta} & 0 \\ \frac{\cos \phi \cos \theta}{r} & \frac{\sin \phi \cos \theta}{r} & -\frac{\sin \theta}{r} \end{bmatrix}.$$

6.12 To solve this problem one could use the transformations (6.33) and the partial derivatives (see Prob. 6.11) to transform by brute force the Laplacian

$$\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

from Cartesian to spherical coordinates and the desired result then would follow straightforwardly.

However, there is a more elegant and “physical” solution of the problem. Let us start from the simple equation (see Eq. (2.134))

$$\begin{aligned}\hat{\mathbf{p}}^2 &= \hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2 \\ &= -\hbar^2 \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) = -\hbar^2 \Delta.\end{aligned}$$

On the other hand, we also have (in the following a summation over repeated indices is understood) (see Eq. (6.3))

$$\begin{aligned}\hat{\mathbf{L}}^2 &= \hbar^2 \hat{\mathbf{I}}^2 = (\hat{\mathbf{r}} \times \hat{\mathbf{p}})^2 = \epsilon_{ijk} \hat{r}_j \hat{p}_k \epsilon_{iab} \hat{r}_a \hat{p}_b \\ &= \hat{r}_j \hat{p}_k \hat{r}_a \hat{p}_b (\epsilon_{ijk} \epsilon_{iab}).\end{aligned}$$

Since $\epsilon_{ijk}\epsilon_{iab} = \delta_{ja}\delta_{kb} - \delta_{jb}\delta_{ka}$, we then have

$$\begin{aligned}\hat{\mathbf{L}}^2 &= \hat{r}_j \hat{p}_k \hat{r}_a \hat{p}_b \delta_{ja} \delta_{kb} - \hat{r}_j \hat{p}_k \hat{r}_a \hat{p}_b \delta_{jb} \delta_{ka} \\ &= \hat{r}_j \hat{p}_k \hat{r}_j \hat{p}_k - \hat{r}_j \hat{p}_k \hat{r}_k \hat{p}_j \\ &= \hat{r}_j (\hat{r}_j \hat{p}_k + [\hat{p}_k, \hat{r}_j]) \hat{p}_k - (\hat{p}_k \hat{r}_j + [\hat{r}_j, \hat{p}_k]) \hat{r}_k \hat{p}_j \\ &= \hat{r}_j (\hat{r}_j \hat{p}_k - \imath \hbar \delta_{jk}) \hat{p}_k - (\hat{p}_k \hat{r}_j + \imath \hbar \delta_{jk}) \hat{r}_k \hat{p}_j \\ &= \hat{r}_j \hat{r}_j \hat{p}_k \hat{p}_k - \imath \hbar \hat{r}_j \hat{p}_j - \hat{p}_k \hat{r}_k \hat{r}_j \hat{p}_j - \imath \hbar \hat{r}_k \hat{p}_k \\ &= \hat{\mathbf{r}}^2 \hat{\mathbf{p}}^2 - \imath \hbar \hat{\mathbf{r}} \cdot \hat{\mathbf{p}} - (\hat{\mathbf{p}} \cdot \hat{\mathbf{r}}) (\hat{\mathbf{r}} \cdot \hat{\mathbf{p}}) - \imath \hbar \hat{\mathbf{r}} \cdot \hat{\mathbf{p}}.\end{aligned}$$

Since $\hat{\mathbf{p}}\hat{\mathbf{r}} = \hat{\mathbf{r}}\hat{\mathbf{p}} - 3\imath\hbar$, we have

$$\begin{aligned}\hat{\mathbf{L}}^2 &= \hat{\mathbf{r}}^2 \hat{\mathbf{p}}^2 - 2\imath \hbar \hat{\mathbf{r}} \cdot \hat{\mathbf{p}} - (\hat{\mathbf{r}} \cdot \hat{\mathbf{p}} - 3\imath \hbar) \hat{\mathbf{r}} \cdot \hat{\mathbf{p}} \\ &= \hat{\mathbf{r}}^2 \hat{\mathbf{p}}^2 - (\hat{\mathbf{r}} \cdot \hat{\mathbf{p}})^2 + \imath \hbar \hat{\mathbf{r}} \cdot \hat{\mathbf{p}}.\end{aligned}$$

On the other hand,

$$\hat{\mathbf{r}} \cdot \hat{\mathbf{p}} = \frac{\hbar}{\imath} \left(x \frac{\partial}{\partial x} + y \frac{\partial}{\partial y} + z \frac{\partial}{\partial z} \right),$$

and, from $r = (x^2 + y^2 + z^2)^{\frac{1}{2}}$,

$$\frac{\partial}{\partial x} = \frac{x}{r} \frac{\partial}{\partial r}, \quad \frac{\partial}{\partial y} = \frac{y}{r} \frac{\partial}{\partial r}, \quad \frac{\partial}{\partial z} = \frac{z}{r} \frac{\partial}{\partial r}.$$

Therefore,

$$\hat{\mathbf{r}} \cdot \hat{\mathbf{p}} = \frac{\hbar}{\imath} r \frac{\partial}{\partial r}.$$

From the previous equations, we obtain

$$\begin{aligned}\hat{\mathbf{p}}^2 &= \frac{1}{r^2} \left[(\hat{\mathbf{r}} \cdot \hat{\mathbf{p}})^2 - \imath \hbar \hat{\mathbf{r}} \cdot \hat{\mathbf{p}} + \hat{\mathbf{L}}^2 \right] \\ &= \hbar^2 \left(-\frac{\partial^2}{\partial r^2} - \frac{2}{r} \frac{\partial}{\partial r} + \frac{\hat{\mathbf{L}}^2}{r^2} \right).\end{aligned}$$

Together with the first equation, we finally obtain

$$\begin{aligned}\Delta &= \frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} - \frac{\hat{\mathbf{L}}^2}{r^2} \\ &= \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) - \frac{\hat{\mathbf{L}}^2}{r^2},\end{aligned}$$

which proves the desired result.

It is interesting to note that the equation

$$\hat{\mathbf{p}}^2 = \frac{1}{r^2} \left[(\hat{\mathbf{r}} \cdot \hat{\mathbf{p}})^2 - \imath \hbar \hat{\mathbf{r}} \cdot \hat{\mathbf{p}} + \hat{\mathbf{L}}^2 \right]$$

bears an important physical meaning: dividing both sides of the equation by $2m$, we have that the total energy of a point-like free quantum particle in the three-dimensional case ($\hat{\mathbf{p}}^2/2m$) may be interpreted as the sum of three terms. The first term, i.e.

$$\frac{(\hat{\mathbf{r}} \cdot \hat{\mathbf{p}})^2}{2mr^2},$$

represents an element of the radial part of the energy. The second term,

$$-\frac{i\hbar \hat{\mathbf{r}} \cdot \hat{\mathbf{p}}}{2mr^2},$$

is a typical quantum-mechanical term that arises from the commutators between position and momentum in the derivation above,⁷ and is the other element of the radial part. The last term, i.e.

$$\frac{\hat{\mathbf{L}}^2}{2mr^2},$$

is the angular part of the total energy.

6.14 We start from Eq. (6.59) and write, for $m = l$ and $m' = l'$,

$$\int d\Omega Y_{l'l'}^*(\phi, \theta) Y_{ll}(\phi, \theta) = \delta_{ll'}.$$

The lhs of the previous equation turns out to be

$$\int_0^{2\pi} d\phi \frac{e^{i(l-l')\phi}}{2\pi} \int_0^\pi d\theta \sin \theta \Theta_{l'l'}^*(\theta) \Theta_{ll}(\theta).$$

Now, since

$$\int_0^{2\pi} d\phi \frac{e^{i(l-l')\phi}}{2\pi} = \delta_{ll'},$$

we must also have

$$I_{ll} = \int_0^\pi d\theta \sin \theta \Theta_{ll}^*(\theta) \Theta_{ll}(\theta) = 1.$$

On the other hand,

$$I_{ll} = |\mathcal{N}|^2 \int_0^\pi d\theta (\sin \theta)^{2l+1} = 2 |\mathcal{N}|^2 \int_0^{\frac{\pi}{2}} d\theta (\sin \theta)^{2l+1}.$$

Since⁸

$$\int_0^{\frac{\pi}{2}} d\theta (\sin \theta)^{2l+1} = \frac{(2l)!!}{(2l+1)!!},$$

then

$$I_{ll} = 2 |\mathcal{N}|^2 \frac{(2l)!!}{(2l+1)!!},$$

from which it follows that

$$|\mathcal{N}| = \sqrt{\frac{(2l+1)!!}{2(2l)!!}} = \frac{1}{2^l l!} \sqrt{\frac{(2l+1)!}{2}}.$$

⁷ This term vanishes in the classical limit $\hbar \rightarrow 0$ (see Pr. 2.3: p. 72).

⁸ See [Gradstein/Ryshik 1981, 3.621.4].

The latter result may be proved by induction (it is trivially true for $l = 1$, and, if it is true for l , it is also true for $l + 1$).

- 6.16** A spherically symmetric Hamiltonian is of the type (6.84). On the other hand, $\hat{\mathbf{I}}^2$ is the angular part of the Laplacian (see Eq. (6.55)). If one bears in mind the explicit expression of the Laplacian in spherical coordinates (Eq. (6.255)), it is clear that

$$[\hat{\mathbf{p}}^2, \hat{\mathbf{I}}^2] = [V(r), \hat{\mathbf{I}}^2] = 0.$$

Concerning \hat{l}_z , we have

$$\begin{aligned} [\hat{\mathbf{p}}^2, \hat{l}_z] &= [\hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2, \hat{x}\hat{p}_y - \hat{y}\hat{p}_x] \\ &= [\hat{p}_x^2, \hat{x}\hat{p}_y] - [\hat{p}_y^2, \hat{y}\hat{p}_x] = [\hat{p}_x^2, \hat{x}]\hat{p}_y - [\hat{p}_y^2, \hat{y}]\hat{p}_x \\ &= -2i\hbar\hat{p}_x\hat{p}_y + 2i\hbar\hat{p}_y\hat{p}_x = 0, \end{aligned}$$

where we have made use of the result of Prob. 2.23. Moreover,

$$\begin{aligned} [\hat{\mathbf{r}}^2, \hat{l}_z] &= [\hat{x}^2 + \hat{y}^2 + \hat{z}^2, \hat{x}\hat{p}_y - \hat{y}\hat{p}_x] \\ &= -[\hat{x}^2, \hat{y}\hat{p}_x] + [\hat{y}^2, \hat{x}\hat{p}_y] = -\hat{y}[\hat{x}^2, \hat{p}_x] + \hat{x}[\hat{y}^2, \hat{p}_y] \\ &= -2i\hbar\hat{y}\hat{x} + 2i\hbar\hat{x}\hat{y} = 0, \end{aligned}$$

where we have made use of the result of Prob. 2.26, and that completes the argument.

- 6.17** We know from Prob. 6.16 that \hat{l}_z commutes with $\hat{\mathbf{p}}^2$ and $\hat{\mathbf{r}}^2$. In turn, this means

$$\begin{aligned} [\hat{l}_z, \hat{p}_x^2 + \hat{p}_y^2] &= [\hat{l}_z, \hat{\mathbf{p}}^2 - \hat{p}_z^2] = 0, \\ [\hat{l}_z, \hat{x}^2 + \hat{y}^2] &= [\hat{l}_z, \hat{\mathbf{r}}^2 - \hat{z}^2] = 0, \end{aligned}$$

since \hat{l}_z commutes with both \hat{p}_z and \hat{z} (see Eq. (6.2c)). This completes the proof.

- 6.20** We explicitly derive the commutation relation $[\hat{\sigma}_x, \hat{\sigma}_y] = 2i\hat{\sigma}_z$ and leave the remaining to the reader. We have

$$\begin{aligned} [\hat{\sigma}_x, \hat{\sigma}_y] &= \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} - \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \\ &= 2i \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \\ &= 2i\hat{\sigma}_z. \end{aligned}$$

- 6.22** We prove the result for $\hat{\sigma}_x$ and leave to the reader the calculation involving $\hat{\sigma}_y$. The characteristic equation for $\hat{\sigma}_x$ is

$$\det(\hat{\sigma}_x - \lambda \hat{I}) = \lambda^2 - 1 = 0,$$

which gives the eigenvalues $\lambda_{1,2} = \pm 1$. We write the eigenvectors as

$$|\uparrow\rangle_x = \begin{pmatrix} a \\ b \end{pmatrix}, \quad \text{and} \quad |\downarrow\rangle_x = \begin{pmatrix} c \\ d \end{pmatrix}.$$

The conditions (6.158a) imply $a = b$ and $d = -c$, so that we finally arrive at the normalized eigenvectors

$$\begin{aligned} |\uparrow\rangle_x &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \left[\begin{pmatrix} 1 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right] = \frac{1}{\sqrt{2}} (|\uparrow\rangle_z + |\downarrow\rangle_z), \\ |\downarrow\rangle_x &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \frac{1}{\sqrt{2}} \left[\begin{pmatrix} 1 \\ 0 \end{pmatrix} - \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right] = \frac{1}{\sqrt{2}} (|\uparrow\rangle_z - |\downarrow\rangle_z). \end{aligned}$$

6.23 It is very easy to show that

$$\hat{\sigma}_z = |\uparrow\rangle_z \langle\uparrow| - |\downarrow\rangle_z \langle\downarrow|.$$

For calculating $\hat{\sigma}_x$ and $\hat{\sigma}_y$, we need to use Eqs. (6.159), that is,

$$\begin{aligned} \hat{\sigma}_x &= \frac{1}{2} (|\uparrow\rangle_x \langle\uparrow| - |\downarrow\rangle_x \langle\downarrow|) \\ &= \frac{1}{2} [(|\uparrow\rangle_z + |\downarrow\rangle_z) ({}_z\langle\uparrow| + {}_z\langle\downarrow|) - (|\uparrow\rangle_z - |\downarrow\rangle_z) ({}_z\langle\uparrow| - {}_z\langle\downarrow|)] \\ &= |\uparrow\rangle_z \langle\downarrow| + |\downarrow\rangle_z \langle\uparrow|, \end{aligned}$$

and

$$\begin{aligned} \hat{\sigma}_y &= \frac{1}{2} (|\uparrow\rangle_y \langle\uparrow| - |\downarrow\rangle_y \langle\downarrow|) \\ &= \frac{1}{2} [(|\uparrow\rangle_z + \iota |\downarrow\rangle_z) ({}_z\langle\uparrow| - \iota {}_z\langle\downarrow|) - (|\uparrow\rangle_z - \iota |\downarrow\rangle_z) ({}_z\langle\uparrow| + \iota {}_z\langle\downarrow|)] \\ &= \iota (-|\uparrow\rangle_z \langle\downarrow| + |\downarrow\rangle_z \langle\uparrow|). \end{aligned}$$

A comparison with the matricial expressions of the vectors $|\uparrow\rangle_z$ and $|\downarrow\rangle_z$ gives immediately the Pauli matrices.

6.24 That Pauli matrices are Hermitian can be immediately recognized by inspection. This property immediately shows that $\hat{\sigma}_j^2 = \hat{I}$ for $j = x, y, z$.

6.25 We proceed as follows:

$$\begin{aligned} (\hat{\sigma} \cdot \mathbf{f})(\hat{\sigma} \cdot \mathbf{f}') &= \hat{\sigma}_j \hat{\sigma}_k f_j f'_k = \left\{ \frac{1}{2} [\hat{\sigma}_j, \hat{\sigma}_k] + \frac{1}{2} [\hat{\sigma}_j, \hat{\sigma}_k]_+ \right\} f_j f'_k \\ &= \left\{ \epsilon_{jkn} \hat{\sigma}_n + \hat{I} \delta_{jk} \right\} f_j f'_k \\ &= \epsilon_{jkn} f_j f'_k \hat{\sigma}_n + \hat{I} \delta_{jk} f_j f'_k \\ &= \epsilon_{jkn} (\mathbf{f} \times \mathbf{f}')_n \hat{\sigma}_n + (\mathbf{f} \cdot \mathbf{f}') \hat{I}. \end{aligned}$$

6.27 It is sufficient to consider the form

$$\left[\frac{1}{2m} \left(p_x + \frac{e}{c} B y \right)^2 - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial y^2} + \frac{p_z^2}{2m} - \tilde{\mu} s_z B - E \right] e^{\frac{i}{\hbar} (p_x x + p_z z)} \varphi(y) = 0.$$

6.28 For the electron we have $g \simeq -2$ (see Eq. (6.169) and comments), and $\tilde{\mu}$ (Eq. (6.173)) becomes

$$\tilde{\mu} = -\frac{e\hbar}{mc}.$$

Therefore, the energy eigenvalues (6.179) may be rewritten as

$$E = \left(n + \frac{1}{2} + s_z\right) \hbar \omega_B + \frac{p_z^2}{2m}.$$

6.29 Given the harmonic-oscillator character of the Schrödinger equation (6.176), we may take full advantage of the eigenfunctions (4.97), with a suitable change of notation. We finally obtain

$$\varphi_n(y) = \left(\frac{m\omega_B}{\pi\hbar}\right)^{\frac{1}{4}} 2^{-\frac{n}{2}} (n!)^{-\frac{1}{2}} e^{-\frac{(y-y_0)^2 m\omega_B}{2\hbar}} H_n \left[(y-y_0) \sqrt{\frac{m\omega_B}{\hbar}}\right].$$

6.30 The first part is trivial. For the second part notice that \hat{l}_z does not commute with $\hat{\mathbf{l}}_{1,2}$.

6.31 We prove the results for the states (6.193c) and (6.194). The derivation for the other two cases is straightforward. Since $\hat{s}_z = \hat{s}_{1z} + \hat{s}_{2z}$ and

$$\hat{s}_{kz} |\uparrow\rangle_{k,z} = \frac{1}{2} |\uparrow\rangle_{k,z} \quad \text{and} \quad \hat{s}_{kz} |\downarrow\rangle_{k,z} = -\frac{1}{2} |\downarrow\rangle_{k,z},$$

we have

$$\begin{aligned} \hat{s}_z |1, 0\rangle_{12} &= \frac{1}{\sqrt{2}} \left[\left(\frac{1}{2} - \frac{1}{2}\right) |\uparrow\rangle_1 |\downarrow\rangle_2 + \left(-\frac{1}{2} + \frac{1}{2}\right) |\downarrow\rangle_1 |\uparrow\rangle_2 \right] = 0, \\ \hat{s}_z |0, 0\rangle_{12} &= \frac{1}{\sqrt{2}} \left[\left(\frac{1}{2} - \frac{1}{2}\right) |\uparrow\rangle_1 |\downarrow\rangle_2 - \left(-\frac{1}{2} + \frac{1}{2}\right) |\downarrow\rangle_1 |\uparrow\rangle_2 \right] = 0. \end{aligned}$$

Concerning the total spin, we first notice that

$$\begin{aligned} \hat{s}^2 &= \hat{s}_1^2 + \hat{s}_2^2 + 2\hat{s}_1 \cdot \hat{s}_2 \\ &= \frac{3}{2} + 2\hat{s}_{1z}\hat{s}_{2z} + \hat{s}_{1+}\hat{s}_{2-} + \hat{s}_{1-}\hat{s}_{2+}, \end{aligned}$$

which can be derived by explicit substitution of $\hat{s}_{1\pm}$, $\hat{s}_{2\pm}$, \hat{s}_1^2 , and \hat{s}_2^2 from Eqs. (6.149) and (6.190). By direct application of the operator \hat{s}^2 above onto the two desired states, we obtain

$$\begin{aligned} \hat{s}^2 |0, 0\rangle_{12} &= 0, \\ \hat{s}^2 |1, 0\rangle_{12} &= 2, \end{aligned}$$

that proves the requested result.

6.34 We know that

$$\begin{aligned} (\Delta\phi)^2 &= \langle \phi^2 \rangle - \langle \phi \rangle^2 \\ &= \int_{-\pi}^{+\pi} d\phi \psi^*(\phi) \phi^2 \psi(\phi) - \left[\int_{-\pi}^{+\pi} d\phi \psi^*(\phi) \phi \psi(\phi) \right]^2. \end{aligned}$$

With the change of variable $\phi + \eta = \xi$, we have

$$\begin{aligned} f(\eta) &= \int_{-\pi}^{+\pi} d\xi \psi^*(\xi) \xi^2 \psi(\xi) + \eta^2 \int_{-\pi}^{+\pi} d\xi \psi^*(\xi) \xi \psi(\xi) - 2\eta \int_{-\pi}^{+\pi} d\xi \psi^*(\xi) \xi \psi(\xi) \\ &= \langle \xi^2 \rangle - 2\eta \langle \xi \rangle + \eta^2. \end{aligned}$$

As a consequence, $f(\eta)$ represents a parabola as a function of η and its minimum value (corresponding to the vertex of the parabola) is obtained for $\eta = \langle \xi \rangle$ and is equal to $\langle \xi^2 \rangle - \langle \xi \rangle^2$, that is to $(\Delta\phi)^2$.

6.35 From the equation

$$(\Delta_\psi O) \cdot (\Delta_\psi O') \geq \frac{1}{2} \left| \langle \psi | [\hat{O}, \hat{O}'] | \psi \rangle \right|,$$

we derive for the uncertainty product of x and y components of the angular momentum, when we suppose to obtain the outcome $\hbar m_j$ in a measurement of \hat{J}_z , the formula

$$(\Delta_\psi J_x) \cdot (\Delta_\psi J_y) \geq \frac{1}{2} \left| \langle \psi | [\hat{J}_x, \hat{J}_y] | \psi \rangle \right| = \frac{\hbar}{2} \langle \psi | \hat{J}_z | \psi \rangle = m_j \frac{\hbar^2}{2}.$$

This result, together with the fact that the maximum value of m is j while the length of the j -vector is $\sqrt{j(j+1)}$, forces us to conclude that the angular momentum vector can never point exactly in the z -direction. Stated in other terms, since the z -direction is arbitrary, the orientation of the angular momentum is always intrinsically uncertain.

It is also possible to derive a finer estimate of the \hat{J}_x and \hat{J}_y uncertainties.⁹ In fact, we have (see Eqs. (2.184))

$$\begin{aligned} \Delta_\psi^2 \hat{J}_x &= \langle \psi | (\hat{J}_x - \langle \hat{J}_x \rangle_\psi)^2 | \psi \rangle \\ &= \langle \hat{J}_x^2 \rangle_\psi - \langle \hat{J}_x \rangle_\psi^2 = \langle \hat{J}_x^2 \rangle_\psi, \end{aligned}$$

and similarly $\Delta_\psi^2 \hat{J}_y = \langle \hat{J}_y^2 \rangle_\psi$. Therefore, we have

$$\begin{aligned} \langle \hat{J}^2 \rangle_\psi &= \langle \hat{J}_x^2 \rangle_\psi + \langle \hat{J}_y^2 \rangle_\psi + \langle \hat{J}_z^2 \rangle_\psi \\ &= \Delta_\psi^2 \hat{J}_x + \Delta_\psi^2 \hat{J}_y + m_j^2. \end{aligned}$$

Since $\langle \hat{J}^2 \rangle_\psi = j(j+1)$, we obtain

$$\Delta_\psi^2 \hat{J}_x + \Delta_\psi^2 \hat{J}_y = j^2 + j - m_j^2.$$

In the case in which $m_j = j$ we have that $\Delta_\psi^2 \hat{J}_x + \Delta_\psi^2 \hat{J}_y = j$.

⁹ See [Edmonds 1957, 18–19].

Chapter 7

7.1 Multiplying Eq. (7.14) on the left by $\langle \mathbf{r}_\delta^{(1)} \mathbf{r}_\eta^{(2)} \mathbf{r}_\zeta^{(3)} |$, it follows that

$$\hat{U}_P^{123} \Psi(\mathbf{r}_\delta^{(1)}, \mathbf{r}_\eta^{(2)}, \mathbf{r}_\zeta^{(3)}) = \Psi(\mathbf{r}_\eta^{(1)} \mathbf{r}_\zeta^{(2)} \mathbf{r}_\delta^{(3)}),$$

where $\Psi(\mathbf{r}_\alpha^{(1)} \mathbf{r}_\beta^{(2)} \mathbf{r}_\gamma^{(3)})$ is the wave function given by the scalar product

$$\Psi(\mathbf{r}_\alpha^{(1)} \mathbf{r}_\beta^{(2)} \mathbf{r}_\gamma^{(3)}) = \langle \mathbf{r}_\alpha^{(1)} \mathbf{r}_\beta^{(2)} \mathbf{r}_\gamma^{(3)} | \Psi \rangle.$$

7.3 It is impossible: it would be a violation of Pauli exclusion principle.

7.6 The position–momentum uncertainty relation (2.190) states that

$$\Delta p_x \Delta x \simeq \hbar.$$

On the other hand,

$$\Delta p_x \simeq \sqrt{p_x^2} \simeq \sqrt{2mE}.$$

Substituting $E = K_B T$ (see Subsec. 1.5.1) in the previous equation, we finally obtain

$$\Delta x \simeq \frac{\hbar}{\sqrt{2mk_B T}},$$

which is the so-called thermal wavelength.

Chapter 8

8.2 The mean value of $\hat{\mathcal{P}}$ calculated on the output state is given by

$$\begin{aligned} \langle \psi' | \hat{\mathcal{P}} | \psi' \rangle &= \frac{1}{2} (\langle 1 | - \iota \langle 2 |) [(1) \langle 1 | - | 2 \rangle \langle 2 |] (| 1 \rangle - \iota | 2 \rangle) \\ &= \frac{1}{2} (1 + \iota) = 0. \end{aligned}$$

The mean value of $\hat{\mathcal{P}}'$ calculated on the input state is given by

$$\begin{aligned} \langle 1 | \hat{\mathcal{P}}' | 1 \rangle &= \langle 1 | \left[\frac{1}{2} (| 1 \rangle - \iota | 2 \rangle) (\langle 1 | + \iota \langle 2 |) - \frac{1}{2} (-\iota | 1 \rangle + | 2 \rangle) (\iota \langle 1 | + \langle 2 |) \right] | 1 \rangle \\ &= \left\langle 1 \left| \frac{1}{2} \right| 1 \right\rangle - \left\langle 1 \left| (-\iota)(\iota) \frac{1}{2} \right| 1 \right\rangle = 0. \end{aligned}$$

8.3 A generic two-dimensional state $|\varphi\rangle$ may be expanded as

$$|\varphi\rangle = \cos \frac{\theta}{2} |1\rangle + e^{i\phi} \sin \frac{\theta}{2} |2\rangle,$$

where θ and ϕ are the polar and azimuthal angles of the Poincaré sphere, respectively. Let us consider the transformation (8.4). The input state $|1\rangle$ corresponds to the north pole, i.e. to $\theta = 0$ (ϕ is not defined). On the contrary, the output state $|\psi'\rangle$ lies on the equator of the Poincaré sphere and corresponds to $\theta = \pi/2$, $\phi = \pi/2$. In a similar way, we can show that the input state $|2\rangle$ (south pole, $\theta = \pi$) is transformed into an equator state ($\theta = \pi/2$). We may then conclude that the considered transformation performs a $\pi/2$ rotation on the polar angle of the Poincaré sphere.

8.4 Consider a transformation \hat{U} such that $|\psi'\rangle = \hat{U}|\psi\rangle$. After some time we shall have $|\psi\rangle \rightarrow |\psi(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}t}|\psi\rangle$ and $|\psi'\rangle \rightarrow |\psi'(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}t}|\psi'\rangle$, \hat{H} being the Hamiltonian of the system. If the symmetry under the transformation \hat{U} must be conserved, then $|\psi'(t)\rangle$ must be also equal to $\hat{U}|\psi(t)\rangle$. Combining the previous equations we obtain on one hand

$$|\psi'(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}t}\hat{U}|\psi\rangle,$$

and, on the other hand,

$$|\psi'(t)\rangle = \hat{U}e^{-\frac{i}{\hbar}\hat{H}t}|\psi\rangle.$$

In conclusion, for the symmetry to be conserved, the operator \hat{U} must commute with the Hamiltonian.

8.5 The hypothesis is that we have $[\hat{O}, \hat{O}'] = i\hbar$ and that \hat{O} and \hat{O}' are unitarily transformed. Then, we have

$$\begin{aligned}\hat{U}\hat{O}\hat{U}^\dagger\hat{U}\hat{O}'\hat{U}^\dagger - \hat{U}\hat{O}'\hat{U}^\dagger\hat{U}\hat{O}\hat{U}^\dagger &= \hat{U}\hat{O}\hat{O}'\hat{U}^\dagger - \hat{U}\hat{O}'\hat{O}\hat{U}^\dagger \\ &= \hat{U}[\hat{O}, \hat{O}']\hat{U}^\dagger \\ &= \hat{U}\hat{U}^\dagger i\hbar = [\hat{O}, \hat{O}'].\end{aligned}$$

You may have recognized that we have already solved this problem in Subsec. 3.5.1.

8.6 It is evident that, if $\hat{U}(a)$ represents a continuous transformation, $a/2$ exists and $\hat{U}(a) = \hat{U}(a/2)\hat{U}(a/2)$. Now, $\hat{U}(a/2)$ can be either unitary or antiunitary. However, the square of both a unitary operator and an antiunitary operator must be a unitary operator (see Properties (8.11)). Therefore, $\hat{U}(a)$ is unitary (see also the Stone theorem: p. 122).

Chapter 9

9.1 After a unitary time-evolution \hat{U}_t , the density matrix $\hat{\rho}_0$ is transformed into

$$\hat{\rho}_t = \hat{U}_t\hat{\rho}_0\hat{U}_t^\dagger,$$

such that

$$\begin{aligned}\hat{\rho}_t^2 &= \hat{U}_t\hat{\rho}_0\hat{U}_t^\dagger\hat{U}_t\hat{\rho}_0\hat{U}_t^\dagger \\ &= \hat{U}_t\hat{\rho}_0^2\hat{U}_t^\dagger,\end{aligned}$$

so that, if $\hat{\rho}_0^2 = \hat{\rho}_0$, then we also have

$$\hat{\rho}_t^2 = \hat{\rho}_t.$$

9.2 The part of $\hat{H}_{S\mathcal{M}}$ related to the system is already diagonal, that is, taking into account the third Pauli's matrix (6.154),

$$1 + \hat{\sigma}_z^S = \begin{bmatrix} 2 & 0 \\ 0 & 0 \end{bmatrix}.$$

Concerning $\hat{\sigma}_x^{\mathcal{M}}$, we calculate the determinant of the first Pauli's matrix

$$\hat{\sigma}_x^{\mathcal{M}} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.$$

Then

$$\det(\hat{\sigma}_x^{\mathcal{M}} - \lambda \hat{I}) = \begin{vmatrix} -\lambda & 1 \\ 1 & -\lambda \end{vmatrix} = \lambda^2 - 1,$$

i.e. $\lambda_{1,2} = \pm 1$. In other words, the action of $\hat{\sigma}_x^{\mathcal{M}}$ on its eigenkets $|\uparrow\rangle_x^{\mathcal{M}}, |\downarrow\rangle_x^{\mathcal{M}}$ is

$$\hat{\sigma}_x^{\mathcal{M}} |\uparrow\rangle_x^{\mathcal{M}} = |\uparrow\rangle_x^{\mathcal{M}}, \quad \hat{\sigma}_x^{\mathcal{M}} |\downarrow\rangle_x^{\mathcal{M}} = -|\downarrow\rangle_x^{\mathcal{M}}.$$

It follows then that (see Eqs. (6.158a) and Prob. 6.22)

$$|\uparrow\rangle_x^{\mathcal{M}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad |\downarrow\rangle_x^{\mathcal{M}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}.$$

9.3 Since a density matrix is a Hermitian operator (see Sec. 5.2), its eigenstates form a basis in the Hilbert space (see Th. 2.2). In this basis it is apparent that the off-diagonal terms of the density matrix are exactly zero.

9.5 We have

$$|\varphi(t)\rangle = \frac{1}{\sqrt{2}} (|\psi_{\uparrow}(t)\rangle |\uparrow\rangle_z + |\psi_{\downarrow}(t)\rangle |\downarrow\rangle_z).$$

In the limit of a perfect overlap between $|\psi_{\uparrow}(t)\rangle$ and $|\psi_{\downarrow}(t)\rangle$, we have $\langle\psi_{\uparrow}(t)|\psi_{\downarrow}(t)\rangle = 1$, and it follows that

$$\hat{\rho}(t) = \frac{1}{2} |\psi(t)\rangle \langle\psi(t)| \begin{pmatrix} 1 & \\ & 1 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ & 1 \end{pmatrix},$$

where $|\psi(t)\rangle = |\psi_{\uparrow}(t)\rangle = |\psi_{\downarrow}(t)\rangle$.

9.6 By making use of the relations (see Eq. (6.147), (4.87), and the first of Eq. (4.85), respectively)

$$\begin{aligned} \frac{1}{2} (1 + \hat{\sigma}_z) |\uparrow\rangle &= |\uparrow\rangle, \\ \hat{a}_1 |0\rangle &= 0, \\ \hat{a}_0 |N\rangle &= \sqrt{N} |N-1\rangle, \end{aligned}$$

we derive

$$\langle\uparrow| \left[N \hat{H}_{SA} \right] |N-1\rangle |\uparrow\rangle = \varepsilon'_{SA} \sqrt{N},$$

which yields

$$\varepsilon'_{SA} \sqrt{N} \tau_0 \simeq 1.$$

9.7 (i) In order to diagonalize the Hamiltonian it suffices to substitute the definitions (9.215) into Eq. (9.61), so as to obtain

$$\hat{H}'_{SA}(\hat{b}) = \frac{1}{2} \frac{\varepsilon_{SA}}{\sqrt{N}} (1 + \hat{\sigma}_z) (\hat{b}_0^\dagger \hat{b}_0 - \hat{b}_1^\dagger \hat{b}_1).$$

The eigenstates of $\hat{H}'_{SA}(\hat{b})$ will be given by

$$|v\rangle_b |\uparrow\rangle = \frac{1}{\sqrt{v!}} \frac{1}{\sqrt{(N-v)!}} (\hat{b}_0^\dagger)^v (\hat{b}_1^\dagger)^{N-v} |0\rangle |\uparrow\rangle,$$

with

$$\hat{H}'_{SA}(\hat{b}) |v\rangle_b |\uparrow\rangle = \frac{\varepsilon_{SA}}{\sqrt{N}} (2v - N) |v\rangle_b |\uparrow\rangle.$$

(ii) Taking advantage of the expression

$$|N\rangle = \frac{1}{\sqrt{N!}} (\hat{a}_0^\dagger)^N |0\rangle,$$

where

$$\hat{a}_0^\dagger = \frac{1}{\sqrt{2}} (\hat{b}_0^\dagger - \hat{b}_1^\dagger),$$

and

$$\begin{aligned} (\hat{a}_0^\dagger)^N &= \left(\frac{1}{\sqrt{2}}\right)^N (\hat{b}_0^\dagger - \hat{b}_1^\dagger)^N \\ &= \left(\frac{1}{\sqrt{2}}\right)^N \sum_{v=0}^N \binom{N}{v} (\hat{b}_0^\dagger)^v (-\hat{b}_1^\dagger)^{N-v}, \end{aligned}$$

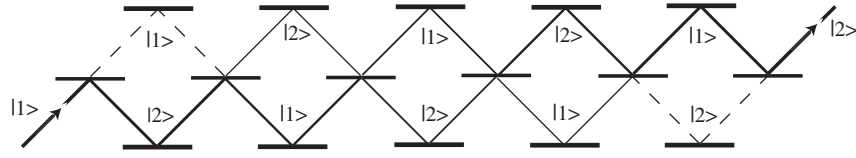
the initial state can be written as

$$\begin{aligned} |\Psi_{SA}(t_0)\rangle &= \left(\frac{1}{\sqrt{2}}\right)^N \sum_{v=0}^N \frac{1}{\sqrt{N!}} \binom{N}{v} (\hat{b}_0^\dagger)^v (-\hat{b}_1^\dagger)^{N-v} |0\rangle |S\rangle \\ &= \left(\frac{1}{\sqrt{2}}\right)^N \sum_{v=0}^N \frac{1}{\sqrt{N!}} \binom{N}{v} (-1)^{N-v} \sqrt{v!} \sqrt{(N-v)!} |v\rangle_b |S\rangle \\ &= \left(\frac{1}{\sqrt{2}}\right)^N \sum_{v=0}^N (-1)^{N-v} \frac{\sqrt{N!}}{\sqrt{v!} (N-v)!} |v\rangle_b |S\rangle. \end{aligned}$$

Inserting this expression into Eq. (9.67) and making use of the above eigenvalue equation for $\hat{H}'_{SA}(\hat{b})$, we obtain

$$\begin{aligned} |\Psi_{SA}(t)\rangle &= c_+ \left[\left(\frac{1}{\sqrt{2}}\right)^N \sum_{v=0}^N (-1)^{N-v} \frac{\sqrt{N!}}{\sqrt{v!} (N-v)!} e^{-\frac{i}{\hbar} \frac{\varepsilon_{SA}}{\sqrt{N}} (2v-N)t} |v\rangle_b \right] |\uparrow\rangle \\ &\quad + c_- |N\rangle |\downarrow\rangle. \end{aligned}$$

In order to obtain the final state (9.68), it is necessary to transform back to the physical states $|a_0\rangle, |a_1\rangle$, i.e. from $|v\rangle_b$ to $|n\rangle$. The transformation is standard but rather cumbersome, and requires some relabeling.



9.8 Stirling's formula states that, for large m ,

$$\ln(m!) \simeq m \ln m - m + \frac{1}{2} \ln m.$$

Taking only the first two (dominant) terms of this expansion, and substituting the resulting approximation

$$m! \simeq m^m e^{-m}$$

into Eq. (9.73), one obtains $\wp_{(m)} \simeq 1$.

9.9 With reference to the above figure, we label by $|1\rangle$ the input state, that is transmitted at the first and at each subsequent beam splitter, and by $|2\rangle$ the state that is reflected at the first beam splitter and then transmitted at each subsequent beam splitter. Using the generic mapping derived in the solution of Prob. 3.12, we may write the transformation at the first beam splitter as

$$|1\rangle \mapsto T|1\rangle + \imath R|2\rangle,$$

where, for the sake of simplicity, we have assumed R and T to be real. The subsequent two mirrors and beam splitter induce the transformations

$$\begin{aligned} T|1\rangle &\mapsto \imath T(T|1\rangle + \imath R|2\rangle), \\ \imath R|2\rangle &\mapsto -R(\imath R|1\rangle + T|2\rangle). \end{aligned}$$

Collecting these results, we have

$$T|1\rangle + \imath R|2\rangle \mapsto \imath(T^2 - R^2)|1\rangle - 2RT|2\rangle.$$

This means that, after two beam splitters, the state has become

$$|\text{out}\rangle_2 = \imath \cos \frac{\pi}{N} |1\rangle - \sin \frac{\pi}{N} |2\rangle,$$

where $R = \cos \pi/2N$ and $T = \sin \pi/2N$. It follows that, after N beam splitters (with N even), we shall have

$$|\text{out}\rangle_N \propto \cos \frac{\pi}{2} |1\rangle + \sin \frac{\pi}{2} |2\rangle = |2\rangle.$$

9.10 In order to prove that $\hat{\rho}_j$ is a density operator it is sufficient to show that $\hat{\rho}_j = \hat{\rho}_j^\dagger$ and $\text{Tr}(\hat{\rho}_j) = 1$.

Since $\hat{\rho}$ is a density operator and therefore $\hat{\rho} = \hat{\rho}^\dagger$, the first condition is immediately verified. In order to verify the second condition we use the cyclic property of the trace and the fact that $\hat{P}_j^2 = \hat{P}_j$ to obtain

$$\text{Tr}(\hat{\rho}_j) = \frac{\text{Tr}(\hat{P}_j \hat{\rho} \hat{P}_j)}{\text{Tr}(\hat{\rho} \hat{P}_j)} = \frac{\text{Tr}(\hat{\rho} \hat{P}_j^2)}{\text{Tr}(\hat{\rho} \hat{P}_j)} = \frac{\text{Tr}(\hat{\rho} \hat{P}_j)}{\text{Tr}(\hat{\rho} \hat{P}_j)} = 1.$$

9.11 In this case we have, using Eq (9.110),

$$\mathcal{T}(\hat{\rho}_i) = |v\rangle \langle v| \hat{\rho}_i |v\rangle \langle v| = \sin^2 \theta |v\rangle \langle v|.$$

Similarly, using the cyclic property of the trace (see Prob. 5.4), we obtain

$$\text{Tr}[\mathcal{T}(\hat{\rho}_i)] = \text{Tr}[\hat{P}_v \hat{\rho}_i \hat{P}_v] = \text{Tr}[\hat{P}_v \hat{\rho}_i] = \langle v | \hat{\rho}_i | v \rangle = \sin^2 \theta,$$

where we have used the obvious fact that $\hat{P}_v^2 = \hat{P}_v$ (see Eq (1.41b)). The desired result immediately follows from the latter two equations.

9.12 The problem can be solved by making repeated use of the cyclic property of the trace and the linearity of the trace operation, that is,

$$\begin{aligned} \text{Tr}[\hat{\rho} \mathcal{T}^*(\hat{O})] &= \text{Tr}\left[\hat{\rho} \sum_k \hat{\vartheta}_k^\dagger \hat{O} \hat{\vartheta}_k\right] \\ &= \text{Tr}\left[\sum_k \hat{\vartheta}_k^\dagger \hat{O} \hat{\vartheta}_k \hat{\rho}\right] \\ &= \sum_k \text{Tr}[\hat{\vartheta}_k^\dagger \hat{O} \hat{\vartheta}_k \hat{\rho}] \\ &= \sum_k \text{Tr}[\hat{O} \hat{\vartheta}_k \hat{\rho} \hat{\vartheta}_k^\dagger] \\ &= \sum_k \text{Tr}[\hat{\vartheta}_k \hat{\rho} \hat{\vartheta}_k^\dagger \hat{O}] \\ &= \text{Tr}\left[\sum_k \hat{\vartheta}_k \hat{\rho} \hat{\vartheta}_k^\dagger\right] \hat{O}. \end{aligned}$$

9.13 From Eq. (9.122) and from the fact that $\text{Tr}[\hat{\rho}_f] = 1$ it follows that

$$\frac{1}{\wp(x_m)} \text{Tr}[\hat{\vartheta}(x_m) \hat{\rho}_i \hat{\vartheta}^\dagger(x_m)] = 1,$$

from which, by the cyclic property of the trace, it further follows that

$$\wp(x_m) = \text{Tr}[\hat{\vartheta}^\dagger(x_m) \hat{\vartheta}(x_m) \hat{\rho}_i].$$

On the other hand, according to Eq. (9.120)

$$\wp(x_m) = \text{Tr}[\hat{E}(x_m) \hat{\rho}_i],$$

and therefore we have

$$\text{Tr}[\hat{\vartheta}^\dagger(x_m) \hat{\vartheta}(x_m) \hat{\rho}_i] = \text{Tr}[\hat{E}(x_m) \hat{\rho}_i].$$

Since the previous equation must hold for any $\hat{\rho}_i$, this implies that $\hat{\vartheta}^\dagger(x_m) \hat{\vartheta}(x_m) = \hat{E}(x_m)$.

9.14 Using expressions (9.125) and (9.127b), we have

$$\begin{aligned}
 \int_{-\infty}^{+\infty} dx_m \wp(x_m) \langle x_S | \hat{\rho}'(x_m) | x_S \rangle &= \int_{-\infty}^{+\infty} dx_m \wp(x_m) \langle x_S | \frac{1}{\wp(x_m)} \hat{E}^{\frac{1}{2}}(x_m) \hat{\rho}_i \hat{E}^{\frac{1}{2}}(x_m) | x_S \rangle \\
 &= \int_{-\infty}^{+\infty} dx_m \langle x_S | \int_{-\infty}^{+\infty} dx'_S [\wp(x_m | x'_S)]^{\frac{1}{2}} | x'_S \rangle \langle x'_S | \\
 &\quad \times \hat{\rho}_i \int_{-\infty}^{+\infty} dx''_S [\wp(x_m | x''_S)]^{\frac{1}{2}} | x''_S \rangle \langle x''_S | x_S \rangle .
 \end{aligned}$$

Given that $\langle x_S | y \rangle = \delta(x_S - y)$, where $|y\rangle$ is an arbitrary eigenstate of \hat{x} , we finally obtain

$$\begin{aligned}
 \int_{-\infty}^{+\infty} dx_m \wp(x_m) \langle x_S | \hat{\rho}'(x_m) | x_S \rangle &= \int_{-\infty}^{+\infty} dx_m \wp(x_m | x_S) \langle x_S | \hat{\rho}_i | x_S \rangle \\
 &= \langle x_S | \hat{\rho}_i | x_S \rangle .
 \end{aligned}$$

9.15 The first beam splitter, the mirror M1, and the phase shifter induce the following transformation on the initial state $|1\rangle$:

$$|1\rangle \xrightarrow{\text{BS1, M1, PS}} \frac{1}{\sqrt{2}} (e^{i\phi} |1\rangle - |2\rangle),$$

which, after the second mirror and BS3, becomes

$$\xrightarrow{\text{M2, BS3}} \frac{1}{\sqrt{2}} \left[\iota e^{i\phi} (\sqrt{\eta} |1\rangle + \iota \sqrt{1-\eta} |3\rangle) - |2\rangle \right].$$

The final state, after BS2, can be written as

$$\begin{aligned}
 |f\rangle &= \frac{1}{\sqrt{2}} \left[\iota e^{i\phi} \sqrt{\eta} \frac{1}{\sqrt{2}} (|1\rangle + \iota |2\rangle) - e^{i\phi} \sqrt{1-\eta} |3\rangle - \frac{1}{\sqrt{2}} (\iota |1\rangle + |2\rangle) \right] \\
 &= \frac{\iota}{2} (e^{i\phi} \sqrt{\eta} - 1) |1\rangle - \frac{1}{2} (e^{i\phi} \sqrt{\eta} + 1) |2\rangle - \frac{e^{i\phi} \sqrt{1-\eta}}{\sqrt{2}} |3\rangle .
 \end{aligned}$$

The detection probabilities can then be calculated as follows:

$$\begin{aligned}
 \wp_1 &= \frac{1}{4} (e^{i\phi} \sqrt{\eta} - 1) (e^{-i\phi} \sqrt{\eta} - 1) \\
 &= \frac{1}{4} (\eta + 1) - \frac{\sqrt{\eta} \cos \phi}{2}, \\
 \wp_2 &= \frac{1}{4} (\eta + 1) + \frac{\sqrt{\eta} \cos \phi}{2}, \\
 \wp_3 &= \frac{1-\eta}{2}.
 \end{aligned}$$

In the case in which $\eta = 1$, we have

$$\begin{aligned}\wp_1 &= \frac{1}{2} (1 - \cos \phi) = \sin^2 \frac{\phi}{2}, \\ \wp_2 &= \frac{1}{2} (1 + \cos \phi) = \cos^2 \frac{\phi}{2}, \\ \wp_3 &= 0,\end{aligned}$$

whereas, when $\eta = 0$, we obtain

$$\begin{aligned}\wp_1 &= \wp_2 = \frac{1}{4}, \\ \wp_3 &= \frac{1}{2}.\end{aligned}$$

9.18 It is easy to show that

$$\begin{aligned}\hat{E}_1 &= \frac{1}{2} \left[\hat{P}_d^{\mathcal{P}} + \eta \hat{P}_u^{\mathcal{P}} - \sqrt{\eta} (\hat{P}_2^{\mathcal{V}} - \hat{P}_1^{\mathcal{V}}) \right] \\ &= \begin{bmatrix} \frac{1}{4} (1 + \eta) - \frac{\sqrt{\eta}}{2} \cos \phi & \frac{1}{4} (1 - \eta) + \iota \frac{\sqrt{\eta}}{2} \sin \phi \\ \frac{1}{4} (1 - \eta) - \iota \frac{\sqrt{\eta}}{2} \sin \phi & \frac{1}{4} (1 + \eta) + \frac{\sqrt{\eta}}{2} \cos \phi \end{bmatrix}, \\ \hat{E}_2 &= \frac{1}{2} \left[\hat{P}_d^{\mathcal{P}} + \eta \hat{P}_u^{\mathcal{P}} + \sqrt{\eta} (\hat{P}_2^{\mathcal{V}} - \hat{P}_1^{\mathcal{V}}) \right] \\ &= \begin{bmatrix} \frac{1}{4} (1 + \eta) + \frac{\sqrt{\eta}}{2} \cos \phi & \frac{1}{4} (1 - \eta) - \iota \frac{\sqrt{\eta}}{2} \sin \phi \\ \frac{1}{4} (1 - \eta) + \iota \frac{\sqrt{\eta}}{2} \sin \phi & \frac{1}{4} (1 + \eta) - \frac{\sqrt{\eta}}{2} \cos \phi \end{bmatrix}, \\ \hat{E}_3 &= (1 - \eta) \hat{P}_u^{\mathcal{P}} = \frac{1 - \eta}{2} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}.\end{aligned}$$

Now, we need to calculate the three expectations for the three detectors, that is

$$\begin{aligned}\wp_1 &= \begin{pmatrix} 1 & 0 \end{pmatrix} \begin{bmatrix} \frac{1}{4} (1 + \eta) - \frac{\sqrt{\eta}}{2} \cos \phi & \frac{1}{4} (1 - \eta) + \iota \frac{\sqrt{\eta}}{2} \sin \phi \\ \frac{1}{4} (1 - \eta) - \iota \frac{\sqrt{\eta}}{2} \sin \phi & \frac{1}{4} (1 + \eta) + \frac{\sqrt{\eta}}{2} \cos \phi \end{bmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ &= \frac{1}{4} (\eta + 1) - \frac{\sqrt{\eta} \cos \phi}{2},\end{aligned}$$

$$\begin{aligned}\wp_2 &= \begin{pmatrix} 1 & 0 \end{pmatrix} \begin{bmatrix} \frac{1}{4} (1 + \eta) + \frac{\sqrt{\eta}}{2} \cos \phi & \frac{1}{4} (1 - \eta) - \iota \frac{\sqrt{\eta}}{2} \sin \phi \\ \frac{1}{4} (1 - \eta) + \iota \frac{\sqrt{\eta}}{2} \sin \phi & \frac{1}{4} (1 + \eta) - \frac{\sqrt{\eta}}{2} \cos \phi \end{bmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ &= \frac{1}{4} (\eta + 1) + \frac{\sqrt{\eta} \cos \phi}{2},\end{aligned}$$

and

$$\begin{aligned}\wp_3 &= \begin{pmatrix} 1 & 0 \end{pmatrix} \frac{1 - \eta}{2} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ &= \frac{1 - \eta}{2},\end{aligned}$$

which fit with the previous calculations.

9.19 The proof of completeness is straightforward. Indeed,

$$\begin{aligned}\hat{E}_1 + \hat{E}_2 + \hat{E}_3 &= \frac{1}{2} \left[\hat{P}_d^{\mathcal{P}} + \eta \hat{P}_u^{\mathcal{P}} - \sqrt{\eta} (\hat{P}_2^{\mathcal{V}} - \hat{P}_1^{\mathcal{V}}) \right] \\ &\quad + \frac{1}{2} \left[\hat{P}_d^{\mathcal{P}} + \eta \hat{P}_u^{\mathcal{P}} + \sqrt{\eta} (\hat{P}_2^{\mathcal{V}} - \hat{P}_1^{\mathcal{V}}) \right] + (1 - \eta) \hat{P}_u^{\mathcal{P}} \\ &= \hat{P}_d^{\mathcal{P}} + \eta \hat{P}_u^{\mathcal{P}} + \hat{P}_u^{\mathcal{P}} - \eta \hat{P}_u^{\mathcal{P}} \\ &= \hat{I}.\end{aligned}$$

The proof of the non-commutability of the above effects is more cumbersome. We here only consider the non-commutability between \hat{E}_1 and \hat{E}_2 . In order to simplify the proof, we take $\eta = 1/2$. Then,

$$\begin{aligned}[\hat{E}_1, \hat{E}_2] &= \frac{1}{4} \left[\frac{2}{\sqrt{2}} (\hat{P}_1^{\mathcal{V}} - \hat{P}_2^{\mathcal{V}}) \hat{P}_d^{\mathcal{P}} - \frac{2}{\sqrt{2}} \hat{P}_d^{\mathcal{P}} (\hat{P}_1^{\mathcal{V}} - \hat{P}_2^{\mathcal{V}}) \right. \\ &\quad \left. - \frac{1}{\sqrt{2}} \hat{P}_u^{\mathcal{P}} (\hat{P}_1^{\mathcal{V}} - \hat{P}_2^{\mathcal{V}}) + \frac{1}{\sqrt{2}} (\hat{P}_1^{\mathcal{V}} - \hat{P}_2^{\mathcal{V}}) \hat{P}_u^{\mathcal{P}} \right] \\ &= \frac{1}{4} \left[\frac{2}{\sqrt{2}} (2\hat{P}_1^{\mathcal{V}} - \hat{I}) \hat{P}_d^{\mathcal{P}} - \frac{2}{\sqrt{2}} \hat{P}_d^{\mathcal{P}} (2\hat{P}_1^{\mathcal{V}} - \hat{I}) \right. \\ &\quad \left. - \frac{1}{\sqrt{2}} \hat{P}_u^{\mathcal{P}} (2\hat{P}_1^{\mathcal{V}} - \hat{I}) + \frac{1}{\sqrt{2}} (2\hat{P}_1^{\mathcal{V}} - \hat{I}) \hat{P}_u^{\mathcal{P}} \right] \\ &= \frac{1}{2\sqrt{2}} (\hat{P}_1^{\mathcal{V}} \hat{P}_d^{\mathcal{P}} - \hat{P}_d^{\mathcal{P}} \hat{P}_1^{\mathcal{V}}),\end{aligned}$$

which, as a direct calculation with the explicit expressions (9.133) and (9.137) of the involved projectors shows, does not vanish (see also Eq. (2.90)). The formal reason for this result lies in the fact that projectors $\hat{P}_1^{\mathcal{V}}$ and $\hat{P}_u^{\mathcal{P}}$ belong to different sets.

9.20 See the original paper [de Muynck *et al.* 1991].

9.21 We are looking for the N functions $\wp_{H_j}(\mathbf{D})$ which make the quantity

$$\langle \mathcal{C} \rangle = \int_{\mathfrak{R}^n} d\mathbf{D} \sum_{j=1}^N R_j(\mathbf{D}) \wp_{H_j}(\mathbf{D})$$

as small as possible. These probability functions are evidently subject to the conditions

$$0 \leq \wp_{H_j}(\mathbf{D}) \leq 1, \quad \sum_{j=1}^N \wp_{H_j}(\mathbf{D}) = 1.$$

It is clear that the average cost will be minimum if the integrand in the rhs of the first equation is chosen to be as small as possible for each data point $\mathbf{D} \in \mathbb{R}^n$. This procedure corresponds to the choice, at each data point \mathbf{D} , of the hypothesis for which the risk $R_j(\mathbf{D})$ is smallest. In practice, at each point \mathbf{D} for which $R_k(\mathbf{D}) < R_j(\mathbf{D})$ ($\forall j \neq k$), we choose

$$\wp_{H_k}(\mathbf{D}) = 1, \quad \wp_{H_j}(\mathbf{D}) = 0.$$

This is the required solution.

In order to render the solution more compact, and to facilitate the comparison with the quantum case, we may also introduce the function

$$L(\mathbf{D}) = \min_j R_j(\mathbf{D}),$$

so that we may rewrite our solution in the form

$$\begin{aligned} [R_j(\mathbf{D}) - L(\mathbf{D})] \wp_{H_j}(\mathbf{D}) &= 0, \\ R_j(\mathbf{D}) - L(\mathbf{D}) &\geq 0. \end{aligned}$$

Finally, note that, by summing the first of the latter two equations over j , the function $L(\mathbf{D})$ may be rewritten as

$$L(\mathbf{D}) = \sum_{j=1}^N R_j(\mathbf{D}) \wp_{H_j}(\mathbf{D}),$$

so that the minimum average cost can be simply expressed as

$$\langle C \rangle_{\min} = \int_{\mathbb{R}^n} d\mathbf{D} L(\mathbf{D}).$$

9.23 In case of binary decision, detection operators commute, since $\hat{E}_{H_1} + \hat{E}_{H_0} = \hat{I}$. The Lagrange operator (see Eq. (9.177)) is given by

$$\hat{L} = \hat{\mathcal{R}}_0 \hat{E}_{H_0} + \hat{\mathcal{R}}_1 \hat{E}_{H_1},$$

and we have

$$\hat{\mathcal{R}}_0 - \hat{L} = \hat{\mathcal{R}}_0 - \hat{\mathcal{R}}_0 \hat{E}_{H_0} - \hat{\mathcal{R}}_1 \hat{E}_{H_1} = (\hat{\mathcal{R}}_0 - \hat{\mathcal{R}}_1) \hat{E}_{H_1}.$$

Eq. (9.178a) now becomes

$$(\hat{\mathcal{R}}_0 - \hat{\mathcal{R}}_1) \hat{E}_{H_1} \hat{E}_{H_0} = 0.$$

Since in general the operator $\hat{\mathcal{R}}_0 - \hat{\mathcal{R}}_1$ does not vanish, we again deal with projectors because \hat{E}_{H_1} and \hat{E}_{H_0} must be orthogonal. In conclusion, in this case the optimal POVM is given by a PVM.

9.24 In view of the symmetry of the expression (9.208), when it is integrated over the hypersphere the terms with $k \neq j$ vanish. Moreover, since $\sum_{k=1}^n |c'_k|^2 = 1$, we have

$$\int_{S_{2n}} d\mathbf{S} |c'_k|^2 = \frac{1}{n} \int_{S_{2n}} d\mathbf{S} \sum_{k=1}^n |c'_k|^2 = \frac{A_{2n}}{n},$$

which proves the result.

9.25 We have

$$\begin{aligned} \langle \varphi | \mathcal{R}_j - \hat{L} | \varphi \rangle &= A_{2n}^{-1} \langle \varphi | \hat{I} - \hat{\rho} | \varphi \rangle \\ &= A_{2n}^{-1} (\langle \varphi | \varphi \rangle - \langle \varphi | \hat{\rho} | \varphi \rangle) \geq 0, \end{aligned}$$

because, for any state $|\varphi\rangle$,

$$\langle \varphi | \hat{\rho} | \varphi \rangle = |\langle \varphi | \psi \rangle|^2 \leq \langle \varphi | \varphi \rangle.$$

Chapter 10

10.1 If the two values of E_l in Eq. (10.27) are equal, we must go to the second order for removing the degeneracy. By multiplying from the left both sides of Eq. (10.9c) by $\langle \psi_q |$ and $\langle \psi_l |$, we obtain

$$\sum'_n c_n^{(1)} \langle \psi_q | \hat{H}' | \psi_n \rangle - d_q E^{(2)} = 0, \quad \sum'_n c_n^{(1)} \langle \psi_l | \hat{H}' | \psi_n \rangle - d_l E^{(2)} = 0,$$

where the prime on the summation symbol denotes omission of the two terms $n = q$ and $n = l$. Substitution of $c_n^{(1)}$ from Eq. (10.30) into the previous equations yields

$$\left(\sum'_n \frac{|\langle \psi_q | \hat{H}' | \psi_n \rangle|^2}{E^{(0)} - E_n^{(0)}} - E^{(2)} \right) d_q + \sum'_n \frac{\langle \psi_q | \hat{H}' | \psi_n \rangle \langle \psi_n | \hat{H}' | \psi_l \rangle}{E^{(0)} - E_n^{(0)}} d_l = 0,$$

$$\sum'_n \frac{\langle \psi_l | \hat{H}' | \psi_n \rangle \langle \psi_n | \hat{H}' | \psi_q \rangle}{E^{(0)} - E_n^{(0)}} d_q + \left(\sum'_n \frac{|\langle \psi_l | \hat{H}' | \psi_n \rangle|^2}{E^{(0)} - E_n^{(0)}} - E^{(2)} \right) d_l = 0.$$

Making use of the argument employed after Eq. (10.27), the analogues of Eqs. (10.28) are

$$\sum'_n \frac{|\langle \psi_q | \hat{H}' | \psi_n \rangle|^2}{E^{(0)} - E_n^{(0)}} = \sum'_n \frac{|\langle \psi_l | \hat{H}' | \psi_n \rangle|^2}{E^{(0)} - E_n^{(0)}}$$

$$\sum'_n \frac{\langle \psi_q | \hat{H}' | \psi_n \rangle \langle \psi_n | \hat{H}' | \psi_l \rangle}{E^{(0)} - E_n^{(0)}} = 0.$$

Unless both of these conditions are satisfied, the degeneracy is removed in second order. A generalization to higher orders and to the cases in which the “ground” state is more than doubly degenerate is straightforward.

10.2 From Eqs. (4.73), we obtain

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} (\hat{a}^\dagger + \hat{a}),$$

and

$$\hat{x}^4 = \left(\frac{\hbar}{2m\omega} \right)^2 \left(\hat{a}^4 + 4\hat{a}^\dagger \hat{a}^3 + 6\hat{a}^2 + 6(\hat{a}^\dagger)^2 \hat{a}^2 + 12\hat{a}^\dagger \hat{a} + 4(\hat{a}^\dagger)^3 \hat{a} + 6(\hat{a}^\dagger)^2 + (\hat{a}^\dagger)^4 + 3 \right),$$

where we have made use of the commutation relation $\hat{a}\hat{a}^\dagger = 1 + \hat{a}^\dagger\hat{a}$ in order to write the annihilation operators to the right of the creation operators.¹⁰ From the

¹⁰ This way of ordering terms involving annihilation and creation operators is called *normal ordering*.

previous equation we immediately infer that $\langle n | \hat{x}^4 | m \rangle$ is different from zero only when $m = n - 4, n - 2, n, n + 2, n + 4$. In particular, we easily obtain

$$\begin{aligned}\langle n | \hat{x}^4 | n \rangle &= \left(\frac{\hbar}{2m\omega} \right)^2 (6n^2 + 6n + 3), \\ \langle n | \hat{x}^4 | n + 2 \rangle &= \left(\frac{\hbar}{2m\omega} \right)^2 (4n + 6) \sqrt{(n + 1)(n + 2)}, \\ \langle n | \hat{x}^4 | n + 4 \rangle &= \left(\frac{\hbar}{2m\omega} \right)^2 \sqrt{(n + 1)(n + 2)(n + 3)(n + 4)}.\end{aligned}$$

In deriving the previous equations we have taken into account that, for example, in the last one only the \hat{a}^4 term survives.

10.3 Starting from Eq. (10.58) and using Eq. (10.62), we have

$$\begin{aligned}c_k^{(1)}(t \geq t_\infty) &= \frac{2 \langle \psi_k | \hat{H}_i' | \psi_l \rangle}{i\hbar} \int_{-\infty}^t dt' e^{i(\omega_{kl} t')} \sin \omega t' \\ &= -\frac{\langle \psi_k | \hat{H}_i' | \psi_l \rangle}{i} \left[\int_0^{t_\infty} dt' e^{i(\omega_{kl} + \omega)t'} - \int_0^{t_\infty} dt' e^{i(\omega_{kl} - \omega)t'} \right] \\ &= -\frac{\langle \psi_k | \hat{H}_i' | \psi_l \rangle}{i\hbar} \left[\frac{e^{i(\omega_{kl} + \omega)t_\infty} - 1}{\omega_{kl} + \omega} - \frac{e^{i(\omega_{kl} - \omega)t_\infty} - 1}{\omega_{kl} - \omega} \right].\end{aligned}$$

10.4 The problem is solved by considering that

$$\begin{aligned}|e^{ixt} - 1|^2 &= (e^{ixt} - 1)(e^{-ixt} - 1) \\ &= 2 - (e^{ixt} + e^{-ixt}) \\ &= 4 \sin^2 \frac{xt}{2}.\end{aligned}$$

10.5 Hamilton equations (1.7) give

$$\dot{x} = \frac{p_x}{m}, \quad \dot{p}_x = -V'(x),$$

where $V(x)$ is the potential energy of the one-dimensional Hamiltonian $H = p_x^2/2m + V(x)$. Then, we have

$$\ddot{x} = \frac{\dot{p}_x}{m} = -\frac{V'(x)}{m} = \frac{f(x)}{m},$$

which is Newton's law. Finally, we obtain

$$\ddot{x} = \frac{\dot{f}(x)}{m} = \frac{1}{m} \frac{df(x)}{dx} \frac{dx}{dt} = \frac{p_x}{m^2} f'(x).$$

10.6 Quantum-mechanically, Eqs. (3.126) and (3.128) give

$$\hat{x} = \frac{\hat{p}_x}{m}, \quad \hat{p}_x = -V'(\hat{x}),$$

from which it follows that

$$\hat{x} = -\frac{1}{m} V'(\hat{x}) = \frac{f(\hat{x})}{m}.$$

Making use of the Heisenberg equation (3.108), we have

$$i\hbar\dot{\hat{x}} = [\hat{x}, \hat{H}] = \frac{1}{m} [f(\hat{x}), \hat{H}] = \frac{1}{2m^2} \left[\frac{f(\hat{x})}{m}, \hat{p}_x^2 \right].$$

Now,

$$\begin{aligned} [f(\hat{x}), \hat{p}_x^2] &= f(\hat{x})\hat{p}_x^2 - \hat{p}_x^2 f(\hat{x}) + \hat{p}_x f(\hat{x})\hat{p}_x - \hat{p}_x f(\hat{x})\hat{p}_x \\ &= [f(\hat{x}), \hat{p}_x] \hat{p}_x + \hat{p}_x [f(\hat{x}), \hat{p}_x] = i\hbar [f'(\hat{x})\hat{p}_x + \hat{p}_x f'(\hat{x})], \end{aligned}$$

where we have taken advantage of the result given in Prob. 2.26. This proves the final result.

10.8 If $V'''(\hat{x})$ is small, according to Eqs. (10.117), one has

$$\begin{aligned} \eta = \langle \hat{H} \rangle - E_c &= \frac{\langle \hat{p}_x^2 \rangle - \langle \hat{p}_x \rangle^2}{2m} + \langle \hat{V} \rangle - V_c \\ &= \frac{1}{2m} (\sigma_p^2 + m\sigma_x^2 V_c'') = \text{const.} \end{aligned}$$

Applying Eq. (3.107) to the operator $\hat{x}^2 - \langle \hat{x} \rangle^2$, one has

$$\begin{aligned} \frac{d}{dt} \sigma_x^2 &= \frac{d}{dt} \langle \hat{x}^2 - \langle \hat{x} \rangle^2 \rangle = \left\langle \frac{d}{dt} (\hat{x}^2 - \langle \hat{x} \rangle^2) \right\rangle \\ &= \frac{1}{m} (\langle \hat{p}_x \hat{x} + \hat{x} \hat{p}_x \rangle - 2\langle \hat{x} \rangle \langle \hat{p}_x \rangle). \end{aligned}$$

Proceeding in a similar way, with $(d/dt)\sigma_x^2$, one obtains

$$\frac{d^2}{dt^2} \sigma_x^2 = \frac{2}{m^2} \sigma_p^2 - \frac{1}{m} (\langle \hat{V}' \hat{x} + \hat{x} \hat{V}' \rangle - 2\langle \hat{x} \rangle \langle \hat{V}' \rangle),$$

where

$$\sigma_p^2 = \langle \hat{p}_x^2 \rangle - \langle \hat{p}_x \rangle^2$$

is the square deviation of \hat{p}_x from its mean. If we replace V' in the last equation with the first two terms of the expansion (10.116b), we arrive at

$$\frac{d^2}{dt^2} \sigma_x^2 \simeq \frac{2}{m^2} (\sigma_p^2 - mV_c'' \sigma_x^2),$$

or, by taking into account that η is constant,

$$\frac{d^2}{dt^2} \sigma_x^2 \simeq \frac{4}{m} (\eta - V_c'' \sigma_x^2).$$

This last equation, within the approximation $V'''(\hat{x}) \simeq 0$, is rather general.

In the case of the free particle, $\langle \hat{x} \rangle$ performs a uniform rectilinear motion with velocity $\langle \hat{p}_x \rangle / m$, and the momentum square deviation remains exactly constant, i.e.

$$\sigma_p^2(t) = \sigma_p^2(t_0) = 2m\eta.$$

Moreover, since

$$\frac{d^2}{dt^2}\sigma_x^2 = \frac{2\sigma_p^2(t_0)}{m^2},$$

one rigorously obtains Eq. (10.119).

Finally, if the free wave packet is taken to be minimum at time t_0 , i.e.

$$\sigma_x^2(t_0) \cdot \sigma_p^2(t_0) = \frac{\hbar}{4},$$

then $\dot{\sigma}_x^2(t_0) = 0$ and

$$\Delta x(t) = \left\{ [\Delta x(t_0)]^2 + \left[\frac{\Delta p_x(t_0)}{m} (t - t_0) \right]^2 \right\}^{\frac{1}{2}}.$$

The second “spreading” term of the rhs of the previous equation allows a classical interpretation of the free wave packet: a bunch of point-like particles-initially contained within a small interval $\Delta x(t_0)$ about the average value $\langle \hat{x}(t_0) \rangle$. Since the velocities of these particles are dispersed over an interval

$$\Delta v_x = \frac{\Delta p_x(t_0)}{m}$$

about the group velocity of the packet

$$v_x = \frac{1}{m} \langle \hat{p}_x(t_0) \rangle,$$

then particles initially located around the same point become uniformly distributed over a band $\Delta v_x \cdot t$ at time t , and the width of the band increases indefinitely.

10.9 The Hamiltonian of the harmonic oscillator is given by Eq. (4.48). Then, Eqs. (10.118) may be rewritten as

$$\frac{d}{dt} \langle \hat{x} \rangle = \frac{\langle \hat{p}_x \rangle}{m} \quad \text{and} \quad \frac{d}{dt} \langle \hat{p}_x \rangle = -m\omega^2 \langle \hat{x} \rangle,$$

which imply

$$\frac{d^2}{dt^2} \langle \hat{x} \rangle = -\omega^2 \langle \hat{x} \rangle \quad \text{and} \quad \frac{d^2}{dt^2} \langle \hat{p}_x \rangle = -\omega^2 \langle \hat{p}_x \rangle,$$

i.e. $\langle \hat{x} \rangle$ and $\langle \hat{p}_x \rangle$ carry out sinusoidal oscillations of frequency $\omega/2\pi$ about the origin. Moreover, we have $V_c'' = m\omega^2$, i.e.

$$\begin{aligned} \eta &= \frac{1}{2m} (\sigma_p^2 + m^2 \omega^2 \sigma_x^2), \\ \frac{d^2}{dt^2} \sigma_x^2 &= \frac{4}{m} \left(\eta - m\omega^2 \sigma_x^2 \right), \\ \frac{d^2}{dt^2} \sigma_p^2 &= 4m\omega^2 \left(\eta - \frac{\sigma_p^2}{m} \right), \end{aligned}$$

which show that σ_x^2 and σ_p^2 oscillate sinusoidally with frequency ω/π about

$$\sigma_x^2 = \frac{\eta}{m\omega^2} \quad \text{and} \quad \sigma_p^2 = m\eta,$$

respectively.

The conditions

$$\frac{d^2}{dt^2}\sigma_x^2 = 0 \quad \text{and} \quad \frac{d^2}{dt^2}\sigma_p^2 = 0$$

require

$$\sigma_x^2 = \frac{\sigma_p^2}{m^2\omega^2},$$

or

$$\eta = \frac{\sigma_p^2}{m} = m\omega^2\sigma_x^2.$$

As we see in Ch. 13, this is equivalent to the condition for a state to be coherent (see Subsec. 13.4.2).

- 10.10** Consider the potential depicted in Fig. 10.4. When $x < x_1$, we have $V(x) = V_0 = \text{const}$. Instead, when $x > x_1$, $V(x)$ is a positive function decreasing monotonically from the positive value $V(x_1)$ to $V(\infty) = 0$. The point of discontinuity x_1 and the turning point x_2 divide the x -axis in regions I, II, and III. In order to find the transmission coefficient, we must construct the solution of the Schrödinger equation whose asymptotic form in region III represents a purely transmitted wave (in the direction of increasing x). In that region, the WKB approximation will have the form (10.134). The condition we impose upon its asymptotic form determines that solution (to within a constant), that is, for $x \gg x_2$,

$$\psi_{\text{III}} = \lambda^{\frac{1}{2}} \left[\cos \left(\int_{x_2}^x dx \frac{1}{\lambda} - i \frac{\pi}{4} \right) + i \sin \left(\int_{x_2}^x dx \frac{1}{\lambda} - \frac{\pi}{4} \right) \right],$$

where the phase $\pi/4$ has been added for the sake of computation. According to Eqs. (10.139), this solution extends to region II (where $x_1 < x \ll x_2$) in the form

$$\psi_{\text{II}} = -i\lambda_q^{\frac{1}{2}} \exp \left(\int_x^{x_2} dx \frac{1}{\lambda_q} \right) = -i\lambda_q^{\frac{1}{2}} e^{\tau} \exp \left(- \int_{x_1}^x dx \frac{1}{\lambda_q} \right),$$

where

$$\tau = \int_{x_1}^{x_2} dx \frac{1}{\lambda_q}.$$

If we define

$$\lambda_q(x_1) = \frac{\hbar}{\sqrt{2m[V(x_1) - E]}} \quad \text{and} \quad k = \frac{\sqrt{2m[E - V_0]}}{\hbar},$$

in region I the solution of the Schrödinger equation may be written

$$\psi_{\text{I}} = C \sin [k(x - x_1) + \delta],$$

where the constants C and δ are obtained applying the continuity conditions to the wave function and its logarithmic derivative at the point x_1 . One then finds that

$$k \cot \delta = -\frac{1}{\lambda_q(x_1)} \quad \text{and} \quad C \sin \delta = -\iota \sqrt{\lambda_q(x_1)} e^\tau.$$

Given these results, one can calculate the transmission probabilities (see also Subsec. 4.2.1). Finally, it should be noted that the present calculation is correct if $V(x)$ varies sufficiently slowly in regions II and III where the WKB approximation has been made. This in turn requires that the barrier be at least several wavelengths thick and that the transmission probability be extremely small ($< 10^{-5}$).

- 10.11** Even though following result can be cast in general terms, we shall limit ourselves to a particle moving in one dimension. Let us start from Eq. (3.99) for the one-dimensional case, i.e.

$$\psi(x', t') = \int dx G(x', t'; x, t) \psi(x, t),$$

where we have omitted the ι factor (see footnote 16, p. 390). In order to derive the desired differential equation, we consider the case in which the time t' is only an infinitesimal interval ϵ after t , i.e. $t' = t + \epsilon$. Taking into account Eq. (10.191) and the fact that for a small time interval ϵ the action is approximately equal to ϵ times the Lagrangian, we have

$$\psi(x, t + \epsilon) = \frac{1}{\mathcal{N}} \int_{-\infty}^{+\infty} dx' e^{\frac{\iota}{\hbar} L\left(\frac{x+x'}{2}, \frac{x-x'}{\epsilon}\right)} \psi(x', t).$$

In the one-dimensional case with a potential $V(x, t)$,

$$L(x, \dot{x}) = \frac{1}{2} m \dot{x}^2 - V(x, t),$$

and

$$\psi(x, t + \epsilon) = \frac{1}{\mathcal{N}} \int_{-\infty}^{+\infty} dx' e^{\frac{\iota}{\hbar} \frac{m(x-x')^2}{2\epsilon}} e^{-\frac{\iota}{\hbar} \epsilon V\left(\frac{x+x'}{2}, t\right)} \psi(x', t).$$

Consider the first exponential in the previous equation: if x' is appreciably different from x , this factor oscillates very rapidly, making the integral over x' vanish. Only for x' values that are close to x do we obtain significant contributions. We therefore make the substitution $x' = x + \eta$, where we expect important contributions only for small values of η . This yields

$$\psi(x, t + \epsilon) = \frac{1}{\mathcal{N}} \int_{-\infty}^{+\infty} d\eta e^{\frac{\iota}{\hbar} \frac{m\eta^2}{2\epsilon}} e^{-\frac{\iota}{\hbar} \epsilon V\left(x + \frac{\eta}{2}, t\right)} \psi(x + \eta, t),$$

where the main contribution to the integral will come from values of η of the order $\sqrt{\epsilon}$. Expanding in power series the lhs up to first order in ϵ and the rhs up to second order in η , we obtain

$$\psi(x, t) + \epsilon \frac{\partial \psi}{\partial t} = \frac{1}{\mathcal{N}} \int_{-\infty}^{+\infty} d\eta e^{\frac{i}{\hbar} \frac{m\eta^2}{2\epsilon}} \left[1 - \frac{i\epsilon}{\hbar} V(x, t) \right] \left[\psi(x, t) + \eta \frac{\partial \psi}{\partial x} + \frac{1}{2} \eta^2 \frac{\partial^2 \psi}{\partial x^2} \right],$$

where we have replaced $\epsilon V(x + \eta/2, t)$ by $\epsilon V(x, t)$, since the error is of order higher than ϵ . Let us consider the leading terms in both sides of the previous equation. We have

$$\psi(x, t) = \psi(x, t) \frac{1}{\mathcal{N}} \int_{-\infty}^{+\infty} d\eta e^{\frac{i}{\hbar} \frac{m\eta^2}{2\epsilon}}.$$

In the limit as ϵ approaches zero, the normalization factor \mathcal{N} must be chosen so that the equality holds. Since¹¹

$$\int_{-\infty}^{+\infty} dx e^{ax^2} = \sqrt{-\frac{\pi}{a}},$$

where a is a complex number, we have

$$\mathcal{N} = \left(\frac{2\pi i \hbar \epsilon}{m} \right)^{\frac{1}{2}}.$$

By making use of the integrals

$$\int_{-\infty}^{+\infty} d\eta e^{\frac{i}{\hbar} \frac{m\eta^2}{2\epsilon}} \eta = 0$$

and¹²

$$\int_{-\infty}^{+\infty} d\eta e^{\frac{i}{\hbar} \frac{m\eta^2}{2\epsilon}} \eta^2 = \frac{i\hbar\epsilon}{m},$$

we finally obtain the equality

$$\psi(x, t) + \epsilon \frac{\partial \psi}{\partial t} = \psi(x, t) - \frac{i\epsilon}{\hbar} V(x, t) \psi(x, t) - \frac{\hbar\epsilon}{2im} \frac{\partial^2 \psi}{\partial x^2}.$$

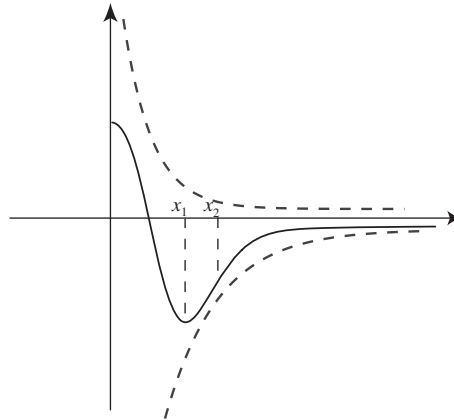
This equality holds to order ϵ if $\psi(x, t)$ satisfies the differential equation

$$i \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x, t) \psi,$$

that is precisely the Schrödinger equation for a one-dimensional system. In a similar way the same result can be obtained in more complicated contexts.

¹¹ [Gradstein/Ryshik 1981, 3.322.2].

¹² [Gradstein/Ryshik 1981, 3.462.8].



Chapter 11

11.4 We have:

$$\lim_{x \rightarrow +\infty} y(x) = 0, \quad \lim_{x \rightarrow 0^+} y(x) = +\infty.$$

Furthermore, studying the first and the second derivatives, we obtain a minimum at (see figure above)

$$x_1 \equiv \left(\frac{2a}{b}; -\frac{b^2}{4a} \right),$$

and a flex at

$$x_2 \equiv \left(\frac{3a}{b}; -\frac{2b^2}{9a} \right).$$

11.5 The reduced mass is given by

$$\begin{aligned} m &= \frac{m_e Z m_p}{m_e + Z m_p} \\ &= m_e \left(1 + \frac{m_e}{Z m_p} \right)^{-1} \\ &\simeq m_e \left(1 - \frac{m_e}{Z m_p} \right), \end{aligned}$$

from which we derive

$$\begin{aligned} \frac{m_e - m}{m_e} &= \frac{\Delta m}{m_e} \\ &\simeq \frac{m_e}{Z m_p}. \end{aligned}$$

In the case of the hydrogen atom ($Z = 1$), we have

$$\frac{\Delta m}{m_e} \simeq 0.05\%.$$

11.6 Starting from Eqs. (11.13c) and (11.18), and making use of substitutions (11.21), (11.23a), and (11.24), we have

$$\begin{aligned}\frac{\hat{H}_I - E_r}{E_0} &= -\frac{1}{E_0} \left[E_r + \frac{\hbar^2}{2m} \frac{\partial^2}{\partial r^2} - \frac{\hbar^2}{2m} \frac{l(l+1)}{r^2} + \frac{Ze^2}{r} \right] \\ &= -\frac{E_r}{E_0} - \frac{\hbar^4}{2m^2 e^4} \frac{\partial^2}{\partial r^2} + \frac{\hbar^4}{2m^2 e^4} \frac{l(l+1)}{r^2} - \frac{\hbar^2}{me^2} \frac{Z}{r} \\ &= -\tilde{E} - \frac{r_0^2}{2} \frac{\partial^2}{\partial r^2} + \frac{r_0^2}{2} \frac{l(l+1)}{r^2} - r_0 \frac{Z}{r} \\ &= -\tilde{E} - \frac{1}{2} \frac{\partial^2}{\partial \tilde{r}^2} + \frac{1}{2} \frac{l(l+1)}{\tilde{r}^2} - \frac{Z}{\tilde{r}},\end{aligned}$$

from which, for $Z = 1$, the desired result can be derived.

11.7 Substituting Eq. (11.27b), i.e.

$$\begin{aligned}\xi''(\tilde{r}) &= \left[-\frac{l+1}{\tilde{r}^2} + \frac{W''}{W} - \frac{(W')^2}{W^2} + \frac{(l+1)^2}{\tilde{r}^2} + \frac{1}{n^2} + \frac{(W')^2}{W^2} \right. \\ &\quad \left. - \frac{2(l+1)}{n\tilde{r}} + \frac{2(l+1)W'}{\tilde{r}W} - \frac{2W'}{nW} \right] \tilde{r}^{l+1} e^{-\frac{\tilde{r}}{n}} W,\end{aligned}$$

and Eq. (11.26), i.e.

$$\tilde{r}^{l+1} e^{-\frac{\tilde{r}}{n}} W(\tilde{r}) = \xi(\tilde{r}),$$

into Eq. (11.23b), we obtain

$$\begin{aligned}0 &= \left[-\frac{l+1}{\tilde{r}^2} + \frac{W''}{W} - \frac{(W')^2}{W^2} + \frac{(l+1)^2}{\tilde{r}^2} + \frac{1}{n^2} + \frac{(W')^2}{W^2} - \frac{2(l+1)}{n\tilde{r}} \right. \\ &\quad \left. + \frac{2(l+1)W'}{\tilde{r}W} - \frac{2W'}{nW} - \frac{1}{n^2} + \frac{2}{\tilde{r}} - \frac{l(l+1)}{\tilde{r}^2} \right] \xi \\ &= \left[\frac{W''}{W} + \left(\frac{2(l+1)}{\tilde{r}} - \frac{2}{n} \right) \frac{W'}{W} + \frac{2}{\tilde{r}} \left(1 - \frac{l+1}{n} \right) \right] \xi.\end{aligned}$$

By multiplying by $W\tilde{r}$, we obtain finally the desired result.

11.8 Consider Eq. (11.30) with $z = -y$, that is,

$$-y \frac{d^2}{d(-y)^2} f(-y) + (\gamma + y) \frac{d}{d(-y)} f(-y) - \alpha f(-y) = 0.$$

It is easy to derive

$$y \frac{d^2}{dy^2} g(y) + (\gamma + y) \frac{d}{d(y)} g(y) + \alpha g(y) = 0,$$

where $g(y) = f(-y)$, which shows that the solution of this equation has the form $g(y) = F(\alpha; \gamma; -y)$. For $y = \eta$ we obtain the result (11.39).

11.9 For each value of n , the possible values of l range from 0 to $n - 1$; moreover, for each value of l there are $2l + 1$ sublevels. The total number of degenerate states is then given by

$$\sum_{l=0}^{n-1} (2l + 1) = \frac{2n(n-1)}{2} + n = n^2,$$

since

$$\sum_{k=0}^m k = \frac{m(m+1)}{2},$$

and

$$\sum_{k=0}^m 1 = m.$$

11.10 We find $R_{10}(\tilde{r})$ and leave the following ones to the reader. In this case, we have $n = 1, l = 0$. As a consequence (see Eq. (11.45)), we have $c_0 = 1, c_1 = 0$, and, for any $j > 1, c_j = 0$. This implies that (see Eq. (11.47)), $W(\eta) = 1$, and (see Eq. (11.26)) $\xi(\tilde{r}) = \tilde{r}e^{-\tilde{r}}$. Finally (see Eq. (11.19)), we obtain

$$R_{10}(\tilde{r}) \propto e^{-\tilde{r}}.$$

11.11 Again, we find the normalization factor for $R_{10}(r)$ and leave the others to the reader. Denoting by \mathcal{N} the normalization factor for $R_{10}(r)$, we must have

$$\mathcal{N}^2 \int_0^{+\infty} dr e^{-2\frac{r}{r_0}} r^2 = 1.$$

Integrating by parts, we obtain

$$\int_0^{+\infty} dx e^{-x} x^2 = 2,$$

which implies

$$2 \left(\frac{r_0}{2} \right)^3 \mathcal{N}^2 = 1,$$

or

$$\mathcal{N} = 2r_0^{-\frac{3}{2}}.$$

11.12 Again, we find the radial probability density corresponding to $R_{10}(r)$ and leave the others to the reader. We have

$$\mathcal{P}_{10}(r) = \frac{4r^2}{r_0^3} e^{-2\frac{r}{r_0}}.$$

11.13 Using the explicit form of the radial wave functions (Eq. (11.51)), we find

$$\begin{aligned}\left\langle \left(\frac{r}{r_0} \right)^2 \right\rangle &= \frac{1}{2} [3n^2 - l(l+1)], \quad \left\langle \frac{r}{r_0} \right\rangle = n^2 [5n^2 + 1 - 3l(l+1)], \\ \left\langle \left(\frac{r}{r_0} \right)^{-1} \right\rangle &= \frac{1}{n^2} \left\langle \left(\frac{r}{r_0} \right)^{-2} \right\rangle = \frac{1}{n^3 \left(l + \frac{1}{2} \right)}, \\ \left\langle \left(\frac{r}{r_0} \right)^{-3} \right\rangle &= \frac{1}{n^3 l \left(l + \frac{1}{2} \right) (l+1)}.\end{aligned}$$

Notice that the latter case is divergent for $l = 0$, but finite for $l > 0$. This is due to the fact that $R(0) \neq 0$ only for $l = 0$, and in this case the radial integral is divergent. The previous results may be used to obtain an interesting consequence. We know that, for a hydrogenoid atom,

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} - \frac{Ze^2}{r},$$

and

$$\langle \hat{V} \rangle = \left\langle -\frac{Ze^2}{r} \right\rangle = -\frac{Ze^2}{r_0} Z \left\langle \left(\frac{r}{r_0} \right)^{-1} \right\rangle = -\frac{Ze^2}{n^2} \frac{mZe^2}{\hbar^2} = 2E_n,$$

where, for a hydrogenoid atom,

$$E_n = -\frac{1}{2}mc^2 \left(\frac{Z\alpha}{n} \right)^2,$$

c is the speed of light, and

$$\alpha = \frac{e^2}{\hbar c} \simeq \frac{1}{137}$$

is the fine-structure constant.

Moreover, the mean value of the kinetic energy becomes

$$\langle \hat{T} \rangle = \langle \hat{H} \rangle - \langle \hat{V} \rangle = E_n - 2E_n = \frac{1}{2}m\langle v^2 \rangle,$$

so that

$$\left\langle \frac{v^2}{c^2} \right\rangle = \frac{2\langle \hat{T} \rangle}{mc^2} = \left(\frac{Z\alpha}{n} \right)^2.$$

For most hydrogenoid atoms this ratio is small because Z is much smaller than 100.

11.14 Impose that the condition

$$\int_0^{+\infty} dr r^2 \int_0^\pi d\theta \sin \theta \int_0^{2\pi} d\phi |\varphi_{nlm}(r, \theta, \phi)|^2 = 1$$

is satisfied for $\varphi_{100}, \varphi_{200}, \varphi_{300}$.

11.15 Make use of Eqs. (6.68)–(6.69) and Eqs. (11.51) and impose the condition of Prob. 11.14.

11.16 The s -levels ($l = 0$) are obviously unaffected by the spin-orbit interaction, since $\hat{\mathbf{l}} \cdot \hat{\mathbf{s}} = 0$ identically.

For the p -levels ($l = 1$), we have either $j = l + 1/2 = 3/2$ or $j = l - 1/2 = 1/2$. In the former case, the energy correction is equal to $\kappa/2$, whereas in the latter it is simply given by $-\kappa$, where $\kappa = \kappa_{l=1}(n)$.

Similarly, for the d -levels ($l = 2$), the correction is equal to $\kappa_{l=2}(n)$ for $j = 5/2$ and to $-3\kappa_{l=2}(n)/2$ for $j = 3/2$.

Finally, for the f -levels ($l = 3$), the correction is equal to $3\kappa_{l=3}(n)/2$ for $j = 7/2$ and to $-2\kappa_{l=3}(n)$ for $j = 5/2$.

It should be noted that the proportionality constant κ grows as Z^4 . As a consequence, the spin-orbit correction is particularly important in the case of heavy atoms. For example, the spin-orbit correction to the $6p$ level of thallium ($Z = 81$, $A = 204$) gives rise to a shift of about 1500 \AA in the wavelength of the radiation emitted in the corresponding transition.

11.21 From the definitions (11.112), we immediately infer that the unit of length is given by r_0 . Moreover, the unit of mass is simply given by the electron mass m_e , and the unit of electron charge is equal to the opposite e of the electron charge. Finally, since the physical dimensions of energy are given by

$$[E] = [m][l]^2[t]^{-2},$$

we obtain

$$m_e \frac{\hbar^4}{m_e^2 e^4} t_0^{-2} = \frac{m_e e^4}{\hbar^2},$$

where t_0 is the atomic unit of time. From this it follows that

$$t_0 = \frac{\hbar^3}{m_e e^4}.$$

11.22 We have

$$\begin{aligned} E_1^{(1)} &= \frac{Z^6}{\pi^2} \int d\mathbf{r}_1 d\mathbf{r}_2 e^{-2Zr_1} e^{-2Zr_2} \frac{1}{r_{12}} \\ &= \frac{Z^6}{\pi^2} \int d\mathbf{r}_1 e^{-2Zr_1} \int dr_2 \int d\cos\theta \frac{2\pi r_2^2 e^{-2Zr_2}}{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos\theta}} \\ &= \frac{Z^6}{\pi^2} 2\pi \int d\mathbf{r}_1 e^{-2Zr_1} \int dr_2 r_2^2 e^{-2Zr_2} \frac{1}{2r_1 r_2} 2\sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos\theta} \Big|_{\cos\theta=1}^{\cos\theta=-1} \\ &= \frac{2Z^6}{\pi} \int d\mathbf{r}_1 e^{-2Zr_1} \int dr_2 r_2 e^{-2Zr_2} \frac{1}{r_1} [(r_1 + r_2) - |r_1 - r_2|] \\ &= \frac{2Z^6}{\pi} \int d\mathbf{r}_1 \frac{e^{-2Zr_1}}{r_1} \left[\int_0^{r_1} dr_2 e^{-2Zr_2} 2r_2^2 + \int_{r_1}^{\infty} dr_2 r_2 e^{-2Zr_2} 2r_1 \right], \end{aligned}$$

where θ is the polar angle. From the previous equation, given that, if $r_2 < r_1$, the second integral in the square brackets is zero, we finally obtain

$$E_1^{(1)} = \frac{2Z^6}{\pi} 16\pi \int_0^\infty dr_1 r_1 \frac{e^{-2Zr_1}}{r_1} \int_0^{r_1} dr_2 e^{-2Zr_2} r_2^2,$$

where the extra factor 2 comes from the contribution of all the symmetric configurations in which $r_2 > r_1$. Now, we compute the previous integral by making use of the expression¹³

$$\int_0^u dx x^n e^{-\mu x} = \frac{n!}{\mu^{n+1}} - e^{-u\mu} \sum_{k=0}^n \frac{n!}{k!} \frac{u^k}{\mu^{n-k+1}},$$

obtaining

$$\begin{aligned} E_1^{(1)} &= 32Z^6 \int d\mathbf{r}_1 e^{-2Zr_1} \left[\frac{2}{(2Z)^3} - e^{-2Zr_1} \left(\frac{2}{(2Z)^3} + \frac{2r_1}{(2Z)^2} + \frac{r_1^2}{2Z} \right) \right] \\ &= \frac{5}{8} Z. \end{aligned}$$

Chapter 12

12.2 The solution of the problem can be found by making use of the mathematical identity

$$\begin{aligned} \nabla^2(fg) &= \nabla [\nabla(fg)] \\ &= \nabla [g\nabla f + f\nabla g] \\ &= g\nabla^2 f + f\nabla^2 g + 2\nabla f \nabla g, \end{aligned}$$

for any pairs of functions $f = f(x, y, z)$ and $g = g(x, y, z)$.

12.3 Given the simplifications (12.16)–(12.21), by making use of the definition (12.10) and of Eqs. (12.11) and (12.13), we obtain

$$\left[-\sum_{k=1}^{N_n} \frac{\hbar^2}{2m_k} \nabla_k^2 + \hat{V}_n + E_e \right] \psi \varphi_{\mathbf{r}_k^n} = \varphi_{\mathbf{r}_k^n} \left[-\sum_{k=1}^{N_n} \frac{\hbar^2}{2m_k} \nabla_k^2 + \hat{V}_n + E_e \right] \psi,$$

from which the result is easily obtained, since the equality

$$\varphi_{\mathbf{r}_k^n} \left[-\sum_{k=1}^{N_n} \frac{\hbar^2}{2m_k} \nabla_k^2 + \hat{V}_n + E_e \right] \psi = E \psi \varphi_{\mathbf{r}_k^n}$$

must hold for any $\varphi_{\mathbf{r}_k^n}$.

12.4 The change of variable (Eq. (12.27)) is equivalent to the following six changes of coordinates:

$$\begin{aligned} x_c &= \frac{m_a x_a^n + m_b x_b^n}{m_a + m_b}, & y_c &= \frac{m_a y_a^n + m_b y_b^n}{m_a + m_b}, & z_c &= \frac{m_a z_a^n + m_b z_b^n}{m_a + m_b}, \\ x_0 &= x_b^n - x_a^n, & y_0 &= y_b^n - y_a^n, & z_0 &= z_b^n - z_a^n, \end{aligned}$$

given $\mathbf{r}_a^n = (x_a^n, y_a^n, z_a^n)$ and $\mathbf{r}_b^n = (x_b^n, y_b^n, z_b^n)$. Limiting ourselves to the x -coordinate, we have

¹³ See [Gradstein/Ryshik 1981, 3.351].

$$\begin{aligned}\frac{\partial}{\partial x_a} &= \frac{\partial x_c}{\partial x_a} \frac{\partial}{\partial x_c} + \frac{\partial x_0}{\partial x_a} \frac{\partial}{\partial x_0} = \frac{m_a}{m_a + m_b} \frac{\partial}{\partial x_c} - \frac{\partial}{\partial x_0}, \\ \frac{\partial}{\partial x_b} &= \frac{\partial x_c}{\partial x_b} \frac{\partial}{\partial x_c} + \frac{\partial x_0}{\partial x_b} \frac{\partial}{\partial x_0} = \frac{m_b}{m_a + m_b} \frac{\partial}{\partial x_c} + \frac{\partial}{\partial x_0},\end{aligned}$$

from which we obtain

$$\begin{aligned}\frac{\partial^2}{\partial x_a^2} &= \frac{m_a^2}{(m_a + m_b)^2} \frac{\partial^2}{\partial x_c^2} + \frac{\partial^2}{\partial x_0^2} - \frac{2m_a}{m_a + m_b} \frac{\partial^2}{\partial x_c \partial x_0}, \\ \frac{\partial^2}{\partial x_b^2} &= \frac{m_b^2}{(m_a + m_b)^2} \frac{\partial^2}{\partial x_c^2} + \frac{\partial^2}{\partial x_0^2} + \frac{2m_b}{m_a + m_b} \frac{\partial^2}{\partial x_c \partial x_0}.\end{aligned}$$

Taking into account only the x -coordinate terms in the Laplacians of Eq. (12.24), we have

$$-\frac{\hbar^2}{2m_a} \frac{\partial^2}{\partial x_a^2} - \frac{\hbar^2}{2m_b} \frac{\partial^2}{\partial x_b^2} = -\frac{\hbar^2}{2(m_a + m_b)} \frac{\partial^2}{\partial x_c^2} - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_0^2}.$$

Adding the similar terms for the y - and z -coordinates, we finally obtain the desired result.

12.5 We may write

$$(\hat{H}_a + \hat{H}_b) \varphi_a(\mathbf{r}_a) \varphi_b(\mathbf{r}_b) = E \varphi_a(\mathbf{r}_a) \varphi_b(\mathbf{r}_b),$$

i.e.

$$\varphi_b(\mathbf{r}_b) \hat{H}_a \varphi_a(\mathbf{r}_a) + \varphi_a(\mathbf{r}_a) \hat{H}_b \varphi_b(\mathbf{r}_b) = E \varphi_a(\mathbf{r}_a) \varphi_b(\mathbf{r}_b).$$

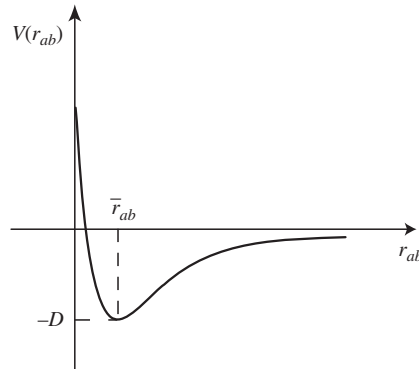
This last equation leads to

$$E = E_a + E_b,$$

provided that we have

$$\begin{aligned}\hat{H}_a \varphi_a(\mathbf{r}_a) &= E_a \varphi_a(\mathbf{r}_a), \\ \hat{H}_b \varphi_b(\mathbf{r}_b) &= E_b \varphi_b(\mathbf{r}_b).\end{aligned}$$

12.8 See the figure below, which represents the Morse potential for a diatomic molecule.



12.9 Just make use of Eq. (12.48) to derive

$$\frac{d}{dr_{ab}} = \frac{d\tilde{r}}{dr_{ab}} \frac{d}{d\tilde{r}} = -a\tilde{r} \frac{d}{d\tilde{r}},$$

and, consequently,

$$\frac{d^2}{dr_{ab}^2} = \frac{d}{dr_{ab}} \frac{d}{dr_{ab}} = a^2 \tilde{r} \left(\frac{d}{d\tilde{r}} + \tilde{r} \frac{d^2}{d\tilde{r}^2} \right).$$

12.11 In order to solve the problem, we need to make use of definitions (12.50), which implies

$$\frac{-2m E_n^{\text{vib}}}{a^2 \hbar^2} = \left[-\left(n + \frac{1}{2}\right) + \frac{\sqrt{2mD}}{a\hbar} \right]^2,$$

from which Eq. (12.55) is easily obtained.

12.12 Let us first rewrite Eq. (12.55) as

$$E_n^{\text{vib}} = -D + \left(n + \frac{1}{2}\right) \hbar a \sqrt{\frac{2D}{m}} - \left(n + \frac{1}{2}\right)^2 \frac{a^2 \hbar^2}{2m},$$

where the last term represents the anharmonic correction of the Morse potential. Comparing the first two terms with Eq. (12.42), we have

$$\omega_0 = a \sqrt{\frac{2D}{m}}.$$

Chapter 13

13.2 Inserting Eqs. (13.3b), (13.9), and (13.8) into Eq. (13.1d), we obtain

$$\nabla \times (\nabla \times \mathbf{A}) = -\frac{1}{c^2} \frac{\partial^2}{\partial t^2} \mathbf{A}.$$

Using the mathematical identity

$$\nabla \times (\nabla \times \mathbf{V}) = \nabla (\nabla \cdot \mathbf{V}) - \nabla^2 \mathbf{V},$$

which holds for any vector \mathbf{V} , and Eq. (13.7), we arrive at

$$\nabla^2 \mathbf{A} = \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \mathbf{A},$$

which is the desired result.

13.4 The expression (13.20a) for $\mathbf{E}(\mathbf{r}, t)$ is calculated using Eq. (13.9) and making use of the expansion

$$\begin{aligned} \hat{\mathbf{A}} = \sum_{\mathbf{k}} c_{\mathbf{k}} l^{-\frac{3}{2}} & \left\{ \left[\hat{a}_{\mathbf{k},1} e^{i\mathbf{k}\cdot\mathbf{r}} e^{-i\omega_{\mathbf{k}} t} + \hat{a}_{\mathbf{k},1}^\dagger e^{-i\mathbf{k}\cdot\mathbf{r}} e^{i\omega_{\mathbf{k}} t} \right] \mathbf{e}_1 \right. \\ & \left. + \left[\hat{a}_{\mathbf{k},2} e^{i\mathbf{k}\cdot\mathbf{r}} e^{-i\omega_{\mathbf{k}} t} + \hat{a}_{\mathbf{k},2}^\dagger e^{-i\mathbf{k}\cdot\mathbf{r}} e^{i\omega_{\mathbf{k}} t} \right] \mathbf{e}_2 \right\}, \end{aligned}$$

from which we obtain easily the desired expression for the electric field. The expression (13.20b) for $\mathbf{B}(\mathbf{r}, t)$ is a bit more cumbersome to derive. We recall the mathematical expression

$$\nabla \times \mathbf{V} = \left(\frac{\partial V_z}{\partial y} - \frac{\partial V_y}{\partial z} \right) \mathbf{i} + \left(\frac{\partial V_x}{\partial z} - \frac{\partial V_z}{\partial x} \right) \mathbf{j} + \left(\frac{\partial V_y}{\partial x} - \frac{\partial V_x}{\partial y} \right) \mathbf{k}$$

for any vector \mathbf{V} , from which, taking into account that

$$e^{i\mathbf{k} \cdot \mathbf{r}} = e^{i(k_x x + k_y y + k_z z)},$$

we have

$$\begin{aligned} \nabla \times (e^{i\mathbf{k} \cdot \mathbf{r}} \mathbf{e}_1) &= i k_z e^{i\mathbf{k} \cdot \mathbf{r}} \mathbf{j} - i k_y e^{i\mathbf{k} \cdot \mathbf{r}} \mathbf{k}, \\ \nabla \times (e^{-i\mathbf{k} \cdot \mathbf{r}} \mathbf{e}_1) &= -i k_z e^{-i\mathbf{k} \cdot \mathbf{r}} \mathbf{j} + i k_y e^{-i\mathbf{k} \cdot \mathbf{r}} \mathbf{k}, \\ \nabla \times (e^{i\mathbf{k} \cdot \mathbf{r}} \mathbf{e}_2) &= -i k_z e^{i\mathbf{k} \cdot \mathbf{r}} \mathbf{i} + i k_x e^{i\mathbf{k} \cdot \mathbf{r}} \mathbf{k}, \\ \nabla \times (e^{-i\mathbf{k} \cdot \mathbf{r}} \mathbf{e}_2) &= +i k_z e^{-i\mathbf{k} \cdot \mathbf{r}} \mathbf{i} - i k_x e^{-i\mathbf{k} \cdot \mathbf{r}} \mathbf{k}. \end{aligned}$$

Collecting these results together, we have

$$\begin{aligned} \nabla \times \hat{\mathbf{A}} &= i \sum_{\mathbf{k}} c'_{\mathbf{k}} \left\{ \left[\hat{a}_{\mathbf{k},1} e^{i(\mathbf{k} \cdot \mathbf{r} - \omega_{\mathbf{k}} t)} - \hat{a}_{\mathbf{k},1}^\dagger e^{-i(\mathbf{k} \cdot \mathbf{r} - \omega_{\mathbf{k}} t)} \right] \mathbf{e}_2 \right. \\ &\quad \left. - \left[\hat{a}_{\mathbf{k},2} e^{i(\mathbf{k} \cdot \mathbf{r} - \omega_{\mathbf{k}} t)} - \hat{a}_{\mathbf{k},2}^\dagger e^{-i(\mathbf{k} \cdot \mathbf{r} - \omega_{\mathbf{k}} t)} \right] \mathbf{e}_1 \right\} \\ &= i \sum_{\mathbf{k}} c'_{\mathbf{k}} \left[\left(\hat{a}_{\mathbf{k},1} e^{i(\mathbf{k} \cdot \mathbf{r} - \omega_{\mathbf{k}} t)} - \hat{a}_{\mathbf{k},1}^\dagger e^{-i(\mathbf{k} \cdot \mathbf{r} - \omega_{\mathbf{k}} t)} \right) \mathbf{b}_1 \right. \\ &\quad \left. + \left(\hat{a}_{\mathbf{k},2} e^{i(\mathbf{k} \cdot \mathbf{r} - \omega_{\mathbf{k}} t)} - \hat{a}_{\mathbf{k},2}^\dagger e^{-i(\mathbf{k} \cdot \mathbf{r} - \omega_{\mathbf{k}} t)} \right) \mathbf{b}_2 \right], \end{aligned}$$

since $k_x = k_y = 0$, $\mathbf{b}_1 = \mathbf{e}_2$ and $\mathbf{b}_2 = -\mathbf{e}_1$ (see Eq. (13.21)), and where

$$c'_{\mathbf{k}} = k_z \left(\frac{\hbar \omega_{\mathbf{k}}}{2\epsilon_0 l^3} \right)^{\frac{1}{2}} = \left(\frac{\hbar k}{2c l^3 \epsilon_0} \right)^{\frac{1}{2}}.$$

13.5 Let us first compute the squares of the electric and magnetic fields

$$\begin{aligned} \hat{\mathbf{E}}^2 &= \sum_{\mathbf{k}, \lambda} \frac{\hbar \omega_{\mathbf{k}}}{2\epsilon_0 l^3} \left[-\hat{a}_{\mathbf{k},\lambda}^2 e^{2i\mathbf{k} \cdot \mathbf{r}} - \left(\hat{a}_{\mathbf{k},\lambda}^\dagger \right)^2 e^{-2i\mathbf{k} \cdot \mathbf{r}} + \hat{a}_{\mathbf{k},\lambda} \hat{a}_{\mathbf{k},\lambda}^\dagger + \hat{a}_{\mathbf{k},\lambda}^\dagger \hat{a}_{\mathbf{k},\lambda} \right], \\ \hat{\mathbf{B}}^2 &= \sum_{\mathbf{k}, \lambda} \frac{\hbar k}{2\epsilon_0 l^3} \left[-\hat{a}_{\mathbf{k},\lambda}^2 e^{2i\mathbf{k} \cdot \mathbf{r}} - \left(\hat{a}_{\mathbf{k},\lambda}^\dagger \right)^2 e^{-2i\mathbf{k} \cdot \mathbf{r}} + \hat{a}_{\mathbf{k},\lambda} \hat{a}_{\mathbf{k},\lambda}^\dagger + \hat{a}_{\mathbf{k},\lambda}^\dagger \hat{a}_{\mathbf{k},\lambda} \right]. \end{aligned}$$

Now, due to the periodic boundary conditions, we have

$$\int_{l^3} d\mathbf{r} e^{2i\mathbf{k} \cdot \mathbf{r}} = 0,$$

since

$$\int_1 dx e^{ik_x x} = \frac{1}{ik_x} e^{i \frac{2\pi n_x}{1} x} \Big|_0^1 = 0,$$

and similarly for the other components.

Substituting these results into Eq. (13.22) and using Eq. (13.2), we obtain Eq. (13.23).

13.6 In order to evaluate the trace in Eq. (13.32) it is easier to work in the energy (number) representation, where

$$\begin{aligned} Z(\beta) &= \sum_{n=0}^{\infty} \langle n | e^{-\beta \hat{H}} | n \rangle = \sum_{n=0}^{\infty} e^{-\beta \hbar \omega (n + \frac{1}{2})} \\ &= e^{-\frac{1}{2} \beta \hbar \omega} \sum_{n=0}^{\infty} (e^{-\beta \hbar \omega})^n = \frac{e^{-\frac{1}{2} \beta \hbar \omega}}{1 - e^{-\beta \hbar \omega}}. \end{aligned}$$

13.7 (a) We have

$$\ln Z = -\frac{1}{2} \beta \hbar \omega - \ln(1 - e^{-\beta \hbar \omega}),$$

and, therefore,

$$\langle E \rangle = -\frac{\partial}{\partial \beta} \ln Z = \frac{1}{2} \hbar \omega + \frac{\hbar \omega}{e^{\beta \hbar \omega} - 1}.$$

(b) The same result can be obtained by making use of the number distribution. In fact, since the energy is diagonal in the number basis, we have

$$\begin{aligned} \langle E \rangle &= \sum_{n=0}^{\infty} E_n \rho_{nn} = \sum_{n=0}^{\infty} \left(n + \frac{1}{2} \right) \hbar \omega \frac{e^{-\beta (n + \frac{1}{2}) \hbar \omega}}{Z(\beta)} \\ &= \frac{\hbar \omega}{2 Z(\beta)} \sum_{n=0}^{\infty} e^{-\beta (n + \frac{1}{2}) \hbar \omega} + \frac{\hbar \omega}{Z(\beta)} \sum_{n=0}^{\infty} n e^{-\beta (n + \frac{1}{2}) \hbar \omega} \\ &= \frac{\hbar \omega}{2} + \hbar \omega (1 - e^{-\beta \hbar \omega}) \sum_{n=0}^{\infty} n e^{-\beta n \hbar \omega} \\ &= \frac{\hbar \omega}{2} + \frac{\hbar \omega}{e^{\beta \hbar \omega} - 1}, \end{aligned}$$

where we have made use of the mathematical relation

$$\sum_{n=0}^{\infty} n x^{n-1} = \frac{d}{dx} \sum_{n=0}^{\infty} x^n = \frac{1}{(1-x)^2}.$$

13.11 Take a generic matrix element of the operators $\widehat{e^{i\phi}}$ and $\widehat{e^{-i\phi}}$ in the number basis. Then, using Eq. (13.39), we have

$$\langle n | \widehat{e^{i\phi}} | m \rangle = \begin{cases} \langle n | m-1 \rangle = \delta_{n,m-1} & \text{for } m \neq 0 \\ 0 & \text{for } m = 0 \end{cases}$$

and

$$\begin{aligned} \langle n | \widehat{e^{-i\phi}} | m \rangle &= \langle n | m+1 \rangle \\ &= \delta_{n,m+1}. \end{aligned}$$

Since for a Hermitian operator \hat{O} we must have $O_{mn} = O_{nm}^*$, we have also proven that $\widehat{e^{i\phi}}$ and $\widehat{e^{-i\phi}}$ are not Hermitian.

13.12 Making use of Eqs. (13.37) and (13.40), we have

$$\begin{aligned}
 [\widehat{\cos\phi}, \widehat{\sin\phi}] &= \frac{1}{4i} \left[(\hat{N}+1)^{-\frac{1}{2}} \hat{a} + \hat{a}^\dagger (\hat{N}+1)^{-\frac{1}{2}} \right] \left[(\hat{N}+1)^{-\frac{1}{2}} \hat{a} - \hat{a}^\dagger (\hat{N}+1)^{-\frac{1}{2}} \right] \\
 &\quad - \frac{1}{4i} \left[(\hat{N}+1)^{-\frac{1}{2}} \hat{a} - \hat{a}^\dagger (\hat{N}+1)^{-\frac{1}{2}} \right] \left[(\hat{N}+1)^{-\frac{1}{2}} \hat{a} + \hat{a}^\dagger (\hat{N}+1)^{-\frac{1}{2}} \right] \\
 &= \frac{1}{2i} \left[-(\hat{N}+1)^{-\frac{1}{2}} \hat{a} \hat{a}^\dagger (\hat{N}+1)^{-\frac{1}{2}} + \hat{a}^\dagger (\hat{N}+1)^{-1} \hat{a} \right] \\
 &= \frac{1}{2i} \left[\hat{a}^\dagger (\hat{N}+1)^{-\frac{1}{2}} (\hat{N}+1)^{-\frac{1}{2}} \hat{a} \right] \\
 &= \frac{1}{2i} [e^{-i\phi}, e^{i\phi}].
 \end{aligned}$$

13.14 In an eigenstate of the number operator we obviously have $\Delta\hat{N} = 0$. We also have

$$\begin{aligned}
 \langle n | \widehat{\cos\phi} | n \rangle &= 0, \\
 \langle n | \widehat{\sin\phi} | n \rangle &= 0.
 \end{aligned}$$

However,

$$\begin{aligned}
 \langle n | \widehat{\cos^2\phi} | n \rangle &= \frac{1}{4} \langle n | e^{i\phi} e^{i\phi} + e^{i\phi} e^{-i\phi} + e^{-i\phi} e^{i\phi} + e^{-i\phi} e^{-i\phi} | n \rangle \\
 &= \begin{cases} \frac{1}{2} & \text{if } n \neq 0 \\ \frac{1}{4} & \text{if } n = 0 \end{cases}.
 \end{aligned}$$

The same values can be derived for $\langle n | \widehat{\sin^2\phi} | n \rangle$. This means that both $\Delta\widehat{\cos\phi}$ and $\Delta\widehat{\sin\phi}$ for $n \neq 0$ are equal to $1/\sqrt{2}$, which confirms that the phase is completely undetermined for an eigenstate of the number operator (i.e. it corresponds to a uniform phase distribution between 0 and 2π).

13.15 By using Eqs. (13.20) and (13.17), one has

$$\hat{\mathbf{E}} = c_B \left\{ \left[\hat{a} e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)} - \hat{a}^\dagger e^{-i(\mathbf{k}\cdot\mathbf{r}-\omega t)} \right] \mathbf{e}_1 + \left[\hat{a} e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)} - \hat{a}^\dagger e^{-i(\mathbf{k}\cdot\mathbf{r}-\omega t)} \right] \mathbf{e}_2 \right\},$$

and

$$\hat{\mathbf{B}} = c_B \left\{ \left[\hat{a} e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)} - \hat{a}^\dagger e^{-i(\mathbf{k}\cdot\mathbf{r}-\omega t)} \right] |\mathbf{k}| \mathbf{e}_2 - \left[\hat{a} e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)} - \hat{a}^\dagger e^{-i(\mathbf{k}\cdot\mathbf{r}-\omega t)} \right] |\mathbf{k}| \mathbf{e}_1 \right\},$$

where

$$c_E = i \left(\frac{\hbar\omega}{2\epsilon_0 l^3} \right)^{\frac{1}{2}} \quad \text{and} \quad c_B = \left(\frac{\hbar k}{2c\epsilon_0 l^3} \right)^{\frac{1}{2}},$$

and we have made use of the fact that

$$\mathbf{b}_1 = \mathbf{k} \times \mathbf{e}_1 = |\mathbf{k}| \mathbf{e}_2 \quad \text{and} \quad \mathbf{b}_2 = \mathbf{k} \times \mathbf{e}_2 = -|\mathbf{k}| \mathbf{e}_1.$$

We also have

$$[\hat{\mathbf{E}}, \hat{\mathbf{B}}] = [\hat{E}_x, \hat{B}_x] + [\hat{E}_y, \hat{B}_y] + [\hat{E}_z, \hat{B}_z].$$

By recalling that the vectors \mathbf{e}_1 and \mathbf{e}_2 are parallel to the x - and y -directions, respectively, and that \mathbf{k} is in the direction of z , the first commutator reads

$$[\hat{E}_x, \hat{B}_x] = \frac{\hbar\omega^2}{2c\epsilon_0 l^3} \left[-(\hat{a} - \hat{a}^\dagger)^2 \right],$$

and similarly for the other commutators.

13.16 The first equation is trivial, since, by using Eq. (13.49a), we immediately obtain

$$\langle \alpha | \hat{a}^\dagger \hat{a} | \alpha \rangle = |\alpha|^2.$$

Analogously, we have

$$\begin{aligned} \langle \hat{N}^2 \rangle_\alpha &= \langle \alpha | \hat{a}^\dagger \hat{a} \hat{a}^\dagger \hat{a} | \alpha \rangle \\ &= |\alpha|^2 \langle \alpha | \hat{a}^\dagger \hat{a} + 1 | \alpha \rangle \\ &= |\alpha|^2 (1 + |\alpha|^2), \end{aligned}$$

from which we obtain

$$\begin{aligned} \Delta_\alpha n &= \sqrt{|\alpha|^2 (1 + |\alpha|^2) - |\alpha|^4} \\ &= \sqrt{|\alpha|^2} = |\alpha|. \end{aligned}$$

13.17 Inverting Eqs. (13.61), we obtain

$$\begin{aligned} \hat{a} &= \frac{1}{\sqrt{2}}(\hat{X}_1 + i\hat{X}_2), \\ \hat{a}^\dagger &= \frac{1}{\sqrt{2}}(\hat{X}_1 - i\hat{X}_2). \end{aligned}$$

Comparing with Eqs. (4.73) we may identify \hat{X}_1 and \hat{X}_2 as

$$\begin{aligned} \hat{X}_1 &= \left(\frac{m\omega}{\hbar} \right)^{\frac{1}{2}} \hat{x}, \\ \hat{X}_2 &= \left(\frac{1}{m\omega\hbar} \right)^{\frac{1}{2}} \hat{p}_x. \end{aligned}$$

13.18 Let us first write an explicit expression for the uncertainties of the quadratures in the coherent state $|\alpha\rangle$. Then we have

$$\begin{aligned} \Delta_\alpha \hat{X}_1 &= \sqrt{\langle \alpha | \hat{X}_1^2 | \alpha \rangle - \left(\langle \alpha | \hat{X}_1 | \alpha \rangle \right)^2} \\ &= \sqrt{\frac{1}{2} \left[\langle \alpha | \hat{a}^2 + \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} + (\hat{a}^\dagger)^2 | \alpha \rangle - \left(\langle \alpha | \hat{a} + \hat{a}^\dagger | \alpha \rangle \right)^2 \right]}, \end{aligned}$$

and

$$\begin{aligned} \Delta_\alpha \hat{X}_2 &= \sqrt{\langle \alpha | \hat{X}_2^2 | \alpha \rangle - \left(\langle \alpha | \hat{X}_2 | \alpha \rangle \right)^2} \\ &= \sqrt{-\frac{1}{2} \left[\langle \alpha | \hat{a}^2 - \hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a} + (\hat{a}^\dagger)^2 | \alpha \rangle - \left(\langle \alpha | \hat{a}^\dagger - \hat{a} | \alpha \rangle \right)^2 \right]}, \end{aligned}$$

where we have made use of Eqs. (13.61). Now we know or may easily derive that

$$\begin{aligned}\langle \alpha | \hat{a} | \alpha \rangle &= \alpha, & \langle \alpha | \hat{a}^\dagger | \alpha \rangle &= \alpha^*, \\ \langle \alpha | \hat{a}^2 | \alpha \rangle &= \alpha^2, & \langle \alpha | (\hat{a}^\dagger)^2 | \alpha \rangle &= (\alpha^*)^2, \\ \langle \alpha | \hat{a}^\dagger \hat{a} | \alpha \rangle &= |\alpha|^2, & \langle \alpha | \hat{a} \hat{a}^\dagger | \alpha \rangle &= 1 + |\alpha|^2.\end{aligned}$$

Making use of these relations, we finally obtain

$$\begin{aligned}\Delta_\alpha \hat{X}_1 &= \sqrt{\frac{1}{2} [(\alpha^2 + 1 + |\alpha|^2 + |\alpha|^2 + (\alpha^*)^2) - (\alpha + \alpha^*)^2]} = \frac{1}{\sqrt{2}} \\ \Delta_\alpha \hat{X}_2 &= \sqrt{-\frac{1}{2} [(\alpha^2 - 1 - |\alpha|^2 - |\alpha|^2 + (\alpha^*)^2) - (\alpha^* - \alpha)^2]} = \frac{1}{\sqrt{2}}.\end{aligned}$$

13.19 To the first order in η we have

$$\begin{aligned}e^{-\eta \hat{\xi}} \hat{\pi} e^{\eta \hat{\xi}} &= (1 - \eta \hat{\xi}) \hat{\pi} (1 + \eta \hat{\xi}) \\ &= \hat{\pi} - \eta [\hat{\xi}, \hat{\pi}].\end{aligned}$$

Similarly, to the second order in η , we may write

$$\begin{aligned}e^{-\eta \hat{\xi}} \hat{\pi} e^{\eta \hat{\xi}} &= \left(1 - \eta \hat{\xi} + \eta^2 \frac{\hat{\xi}^2}{2}\right) \hat{\pi} \left(1 + \eta \hat{\xi} + \eta^2 \frac{\hat{\xi}^2}{2}\right) \\ &= \hat{\pi} - \eta [\hat{\xi}, \hat{\pi}] + \eta^2 \frac{\hat{\xi}^2}{2} \hat{\pi} - \eta^2 \hat{\xi} \hat{\pi} \hat{\xi} + \eta^2 \hat{\pi} \frac{\hat{\xi}^2}{2}.\end{aligned}$$

Now, we have that

$$\begin{aligned}[\hat{\xi}, [\hat{\xi}, \hat{\pi}]] &= [\hat{\xi}, \hat{\xi} \hat{\pi} - \hat{\pi} \hat{\xi}] \\ &= \hat{\xi}^2 \hat{\pi} - 2\hat{\xi} \hat{\pi} \hat{\xi} + \hat{\pi} \hat{\xi}^2,\end{aligned}$$

from which Eq. (13.232) follows to the second order in η .

For the proof of the general result, let us first compute the derivative of the lhs of Eq. (13.232) with respect to η , that is,

$$\frac{d}{d\eta} e^{-\eta \hat{\xi}} \hat{\pi} e^{\eta \hat{\xi}} = -\hat{\xi} e^{-\eta \hat{\xi}} \hat{\pi} e^{\eta \hat{\xi}} + e^{-\eta \hat{\xi}} \hat{\pi} e^{\eta \hat{\xi}} \hat{\xi}.$$

Let us make use of the substitution $\hat{O} \equiv e^{-\eta \hat{\xi}} \hat{\pi} e^{\eta \hat{\xi}}$. Then, the previous equation reads as

$$\frac{d\hat{O}}{d\eta} = [\hat{O}, \hat{\xi}].$$

If we denote the rhs of Eq. (13.232) as \hat{O}' , we easily see that, by computing again the derivative with respect to η ,

$$\frac{d\hat{O}'}{d\eta} = [\hat{O}', \hat{\xi}].$$

Now, the last two equations show that \hat{O} and \hat{O}' satisfy the same differential equation. As a consequence, for any boundary condition $\hat{O} \equiv \hat{O}'$ and the lhs and the rhs of Eq. (13.232) are equal.

13.20 Let us first write¹⁴

$$\hat{\xi}(\eta) = e^{\eta\hat{O}} e^{\eta\hat{O}'},$$

and compute its derivative with respect to η :

$$\begin{aligned} \frac{d}{d\eta} \hat{\xi}(\eta) &= \hat{O} e^{\eta\hat{O}} e^{\eta\hat{O}'} + e^{\eta\hat{O}} \hat{O}' e^{\eta\hat{O}'} \\ &= (\hat{O} + e^{\eta\hat{O}} \hat{O}' e^{-\eta\hat{O}}) \hat{\xi}(\eta). \end{aligned}$$

However, by making use of the results of Prob. 13.19 and of the fact that

$$[\hat{O}, [\hat{O}, \hat{O}']] = [\hat{O}', [\hat{O}, \hat{O}']] = 0,$$

we obtain

$$e^{\eta\hat{O}} \hat{O}' e^{-\eta\hat{O}} = \hat{O}' - \eta [\hat{O}', \hat{O}],$$

which implies

$$\frac{d}{d\eta} \hat{\xi}(\eta) = (\hat{O} + \hat{O}' + \eta [\hat{O}, \hat{O}']) \hat{\xi}(\eta).$$

$\hat{\xi}(\eta)$ is the solution of this differential equation for which $\hat{\xi}(0) = 1$. Since the commutator $[\hat{O}', \hat{O}]$ commutes with $(\hat{O} + \hat{O}')$, by integrating the previous equation, we finally obtain

$$\hat{\xi}(\eta) = e^{\eta(\hat{O} + \hat{O}')} e^{\frac{\eta^2}{2} [\hat{O}, \hat{O}']},$$

which, for $\eta = 1$, proves the desired result.

13.23 Let us consider an initial coherent state $|\alpha\rangle$. Its time evolution is given by

$$|\alpha, t\rangle = e^{-\frac{i}{\hbar} \hat{H}t} |\alpha\rangle,$$

where

$$\hat{H} = \hbar\omega \left(\hat{a}^\dagger \hat{a} + \frac{1}{2} \right)$$

is the single-mode free-field harmonic-oscillator Hamiltonian. We want now to verify that $|\alpha, t\rangle$ is an eigenstate of the annihilation operator. We have

$$\hat{a} |\alpha, t\rangle = \hat{a} e^{-\frac{i}{\hbar} \hat{H}t} |\alpha\rangle = e^{-\frac{i}{\hbar} \hat{H}t} e^{+\frac{i}{\hbar} \hat{H}t} \hat{a} e^{-\frac{i}{\hbar} \hat{H}t} |\alpha\rangle.$$

To evaluate $e^{+\frac{i}{\hbar} \hat{H}t} \hat{a} e^{-\frac{i}{\hbar} \hat{H}t}$ we use the formula (13.234),

$$e^{-\hat{O}} \hat{O}' e^{\hat{O}} = \sum_n \frac{(-1)^n}{n!} [\hat{O}, \hat{O}']_n.$$

¹⁴ See [Gardiner 1991, 138–39] and [Messiah 1958, 442].

The evaluation of the first two terms of the infinite sum in the formula above with $\hat{O} = -i\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)t$ and $\hat{O}' = \hat{a}$ allows us to write

$$e^{+\frac{i}{\hbar}\hat{H}t}\hat{a}e^{-\frac{i}{\hbar}\hat{H}t} = \sum_n \frac{(-i\omega t)^n}{n!}\hat{a} = \hat{a}e^{-i\omega t},$$

where we have also made use of the result of Prob. 4.11. Using this result, we obtain

$$\begin{aligned}\hat{a}|\alpha, t\rangle &= e^{-\frac{i}{\hbar}\hat{H}t}e^{-i\omega t}\hat{a}|\alpha\rangle = \alpha e^{-i\omega t}e^{-\frac{i}{\hbar}\hat{H}t}|\alpha\rangle \\ &= \alpha e^{-i\omega t}|\alpha, t\rangle,\end{aligned}$$

which shows that the initial coherent state $|\alpha\rangle$ under time evolution remains a coherent state, i.e. the state $|\alpha, t\rangle = |\alpha(t)\rangle$ with eigenvalue $\alpha(t) = \alpha e^{-i\omega t}$.

- 13.24** Using the completeness relation (13.71) we have, for any state $|\psi_F\rangle$ of the radiation field,

$$|\psi_F\rangle = \frac{1}{\pi} \int d^2\alpha |\alpha\rangle \langle\alpha| \psi_F\rangle.$$

In particular, for a generic coherent state $|\beta\rangle$ we have

$$\begin{aligned}|\beta\rangle &= \frac{1}{\pi} \int d^2\alpha \langle\alpha| \beta\rangle |\alpha\rangle \\ &= \frac{1}{\pi} e^{-\frac{1}{2}|\beta|^2} \int d^2\alpha e^{\alpha^*\beta - \frac{1}{2}|\alpha|^2} |\alpha\rangle,\end{aligned}$$

where we have made use of expression (13.69).

- 13.27** Given the most general expression of the density matrix $\hat{\rho} = \sum_j w_j |\psi_j\rangle\langle\psi_j|$ with $\sum_j w_j = 1$ (see Eq. (5.20)) and $\{|\psi_j\rangle\}$ representing an orthonormal basis, we may write

$$Q(\alpha, \alpha^*) = \frac{1}{\pi} \sum_j w_j |\langle\alpha| \psi_j\rangle|^2 \leq \frac{1}{\pi} \sum_j w_j = \frac{1}{\pi},$$

since $|\langle\alpha| \psi_j\rangle|^2 \leq 1$.

- 13.28** Any density matrix may be written as $\hat{\rho} = \sum_j w_j |\psi_j\rangle\langle\psi_j|$, $\{|\psi_j\rangle\}$ representing an orthonormal basis. On the other hand we have $\sum_j w_j = 1$. Then, we may write

$$\begin{aligned}|\langle n|\hat{\rho}|m\rangle| &= \left| \sum_j w_j \langle n|\psi_j\rangle\langle\psi_j|m\rangle \right| \\ &\leq \sum_j w_j |\langle n|\psi_j\rangle| |\langle\psi_j|m\rangle|.\end{aligned}$$

Making use of the fact that, for any real x and y , $2xy \leq x^2 + y^2$, we have

$$\begin{aligned}\sum_j w_j |\langle n|\psi_j\rangle| |\langle\psi_j|m\rangle| &\leq \sum_j \frac{1}{2} w_j \left[|\langle n|\psi_j\rangle|^2 + |\langle\psi_j|m\rangle|^2 \right] \\ &= \frac{1}{2} \left[\sum_j w_j |\langle n|\psi_j\rangle|^2 + \sum_j w_j |\langle\psi_j|m\rangle|^2 \right].\end{aligned}$$

Since

$$|\langle n | \psi_j \rangle|^2 \leq 1 \quad \text{and} \quad |\langle \psi_j | m \rangle|^2 \leq 1,$$

we finally have

$$\frac{1}{2} \left[\sum_j w_j |\langle n | \psi_j \rangle|^2 + \sum_j w_j |\langle \psi_j | m \rangle|^2 \right] \leq \frac{1}{2} \left(2 \sum_j w_j \right) = 1.$$

13.30 Using the identity

$$\frac{1}{2\pi} \int_{-\infty}^{+\infty} dx e^{ixy} = \delta(y),$$

we have

$$\begin{aligned} \int_{-\infty}^{+\infty} dp_x W(x, p_x) &= \frac{1}{\pi h} \int_{-\infty}^{+\infty} dx' \langle x + x' | \hat{\rho} | x - x' \rangle \int_{-\infty}^{+\infty} dp_x e^{2i \frac{p_x x'}{h}} \\ &= \langle x | \hat{\rho} | x \rangle = \wp(x). \end{aligned}$$

Chapter 14

14.1 Let us write $|R\rangle = \sum_j a_j |r_j\rangle$, $|R_0\rangle = \sum_j a_j^0 |r_j\rangle$, and $|R_1\rangle = \sum_j a_j^1 |r_j\rangle$.

Then, we have

$$\begin{aligned} \hat{\rho}^{\mathcal{SR}} &= |c_0|^2 |0\rangle \langle 0| \sum_{n,j} a_n^0 (a_j^0)^* |r_n\rangle \langle r_j| + |c_1|^2 |1\rangle \langle 1| \sum_{n,j} a_n^1 (a_j^1)^* |r_n\rangle \langle r_j| \\ &\quad + c_0 c_1^* |0\rangle \langle 1| \sum_{n,j} a_n^0 (a_j^1)^* |r_n\rangle \langle r_j| + c_0^* c_1 |1\rangle \langle 0| \sum_{n,j} a_n^1 (a_j^0)^* |r_n\rangle \langle r_j|. \end{aligned}$$

Now, by tracing the reservoir out, we obtain the reduced density matrix

$$\begin{aligned} \hat{\rho}^{\mathcal{S}} &= \sum_k \langle r_k | \hat{\rho}^{\mathcal{SR}} | r_k \rangle \\ &= |c_0|^2 |0\rangle \langle 0| \sum_n |a_n^0|^2 + |c_1|^2 |1\rangle \langle 1| \sum_n |a_n^1|^2 \\ &\quad + c_0 c_1^* |0\rangle \langle 1| \sum_n a_n^0 (a_n^1)^* + c_0^* c_1 |1\rangle \langle 0| \sum_n a_n^1 (a_n^0)^*. \end{aligned}$$

The sums $\sum_n |a_n^0|^2$ and $\sum_n |a_n^1|^2$ are the traces of \hat{P}_0 and \hat{P}_1 , respectively, where

$$\hat{P}_0 = |R_0\rangle \langle R_0| = \sum_{n,j} a_n^0 (a_j^0)^* |r_n\rangle \langle r_j|, \quad \hat{P}_1 = |R_1\rangle \langle R_1| = \sum_{n,j} a_n^1 (a_j^1)^* |r_n\rangle \langle r_j|,$$

and, by the normalization condition, both are equal to 1. The terms $\sum_n a_n^0 (a_n^1)^*$ and $\sum_n a_n^1 (a_n^0)^*$ are equal to $\langle R_1 | R_0 \rangle$ and $\langle R_0 | R_1 \rangle$, respectively. In fact,

$$\begin{aligned} \langle R_1 | R_0 \rangle &= \sum_{n,j} a_n^0 (a_j^1)^* \langle r_j | r_n \rangle = \sum_n a_n^0 (a_n^1)^*, \\ \langle R_0 | R_1 \rangle &= \sum_{n,j} a_n^1 (a_j^0)^* \langle r_j | r_n \rangle = \sum_n a_n^1 (a_n^0)^*. \end{aligned}$$

Collecting these results and writing them in matrix form, we obtain Eq. (14.5).

14.2 It is easy to see that

$$\begin{aligned} \left\{ \hat{O} \left| \hat{O}' \right. \right\} &= \sum_{l,m,j,k} O_{l,m}^* O'_{j,k} \{l,m|j,k\} = O_{l,m}^* O'_{j,k} \delta_{l,j} \delta_{k,m} \\ &= \sum_{l,m} O_{l,m}^* O'_{l,m} = \sum_{l,m} O_{ml}^\dagger O'_{l,m} = \text{Tr}(\hat{O}^\dagger \hat{O}'), \end{aligned}$$

and

$$\begin{aligned} \{j,k|\hat{O}\} &= \{j,k|\sum_{l,m} O_{l,m}|l,m\rangle\rangle \\ &= \sum_{l,m} O_{l,m} \delta_{l,j} \delta_{k,m} = O_{j,k}. \end{aligned}$$

14.5 Let us write the density matrix $\hat{\rho}$ in terms of the expansion (13.92), that is,

$$\hat{\rho} = \pi \sum_{n,m} Q_{n,m} (\hat{a}^\dagger)^n \hat{a}^m.$$

Then, we may write

$$\begin{aligned} \hat{\rho} \hat{a}^\dagger &= \pi \sum_{n,m} Q_{n,m} (\hat{a}^\dagger)^n \hat{a}^m \hat{a}^\dagger \\ &= \hat{a}^\dagger \pi \sum_{n,m} Q_{n,m} (\hat{a}^\dagger)^n \hat{a}^m + \pi \sum_{n,m} m Q_{n,m} (\hat{a}^\dagger)^n \hat{a}^{m-1} \\ &= \hat{a}^\dagger \hat{\rho} + \frac{d\hat{\rho}}{d\hat{a}}, \end{aligned}$$

where we have taken into account the result

$$\hat{a}^m \hat{a}^\dagger = \hat{a}^\dagger \hat{a}^m + m \hat{a}^{m-1}$$

of Prob. 4.12. The final equality on the rhs of Eq. (14.53) may be derived by taking into account the expansion (13.91) that yields

$$\left\langle \alpha \left| \frac{d\hat{\rho}}{d\hat{a}} \right| \alpha \right\rangle = \pi \frac{\partial Q}{\partial \alpha}.$$

14.6 We have that

$$\left\langle \alpha \left| \hat{a} \hat{\rho} \hat{a}^\dagger \right| \alpha \right\rangle = \left\langle \alpha \left| \hat{a}^\dagger \hat{\rho} \hat{a} + \hat{a}^\dagger \frac{d\hat{\rho}}{d\hat{a}^\dagger} + \hat{\rho} + \frac{d\hat{\rho}}{d\hat{a}} \hat{a} + \frac{d^2 \hat{\rho}}{d\hat{a} d\hat{a}^\dagger} \right| \alpha \right\rangle,$$

since

$$\hat{\rho} \hat{a}^\dagger = \hat{a}^\dagger \hat{\rho} + \frac{d\hat{\rho}}{d\hat{a}} \quad \text{and} \quad \hat{a} \hat{\rho} = \hat{\rho} \hat{a} + \frac{d\hat{\rho}}{d\hat{a}^\dagger}.$$

By making use of the previous results we obtain the desired solution.

14.8 We have that

$$\begin{aligned}
 \mathbf{s}^2 &= s_x^2 + s_y^2 + s_z^2 \\
 &= \rho_{eg}^2 + \rho_{ge}^2 + 2\rho_{eg}\rho_{ge} - \rho_{eg}^2 - \rho_{ge}^2 + 2\rho_{eg}\rho_{ge} + \rho_{ee}^2 + \rho_{gg}^2 - 2\rho_{ee}\rho_{gg} \\
 &= \rho_{ee}^2 + \rho_{gg}^2 + 4\rho_{eg}\rho_{ge} - 4\rho_{ee}\rho_{gg} + 2\rho_{ee}\rho_{gg} \\
 &= 1 + 4(\rho_{eg}\rho_{ge} - \rho_{ee}\rho_{gg}),
 \end{aligned}$$

where we have made use of the fact that, since $\rho_{ee} + \rho_{gg} = 1$ (they are the diagonal elements of the density matrix), also $\rho_{ee}^2 + \rho_{gg}^2 + 2\rho_{ee}\rho_{gg} = 1$. Now it is easy to show that $1 + 4(\rho_{eg}\rho_{ge} - \rho_{ee}\rho_{gg})$ is equal to one in the case of pure states and strictly smaller than 1 in the case of mixtures. In fact, if $\hat{\rho}$ is a pure state, we must have that $\text{Tr}(\hat{\rho}^2) = 1$. This means that the sum of the diagonal elements of $\hat{\rho}^2$ must be equal to 1, i.e.

$$\rho_{gg}^2 + \rho_{ge}\rho_{eg} + \rho_{eg}\rho_{ge} + \rho_{ee}^2 = 1,$$

from which it follows that

$$\rho_{ge}\rho_{eg} = \rho_{ee}\rho_{gg},$$

which immediately gives the desired result.

In the case in which $\hat{\rho}$ is a mixture, we have that $\text{Tr}(\hat{\rho}^2) < 1$, and, therefore, we also must have that

$$\rho_{gg}^2 + \rho_{ge}\rho_{eg} + \rho_{eg}\rho_{ge} + \rho_{ee}^2 < 1,$$

from which it follows that

$$\rho_{ge}\rho_{eg} < \rho_{ee}\rho_{gg},$$

from which it follows that $1 + 4(\rho_{eg}\rho_{ge} - \rho_{ee}\rho_{gg}) < 1$.

14.9 We recall that

$$\begin{aligned}
 \hat{\sigma}_- |e\rangle &= |g\rangle, \quad \hat{\sigma}_- |g\rangle = 0, \\
 \hat{\sigma}_+ |e\rangle &= 0, \quad \hat{\sigma}_+ |g\rangle = |e\rangle.
 \end{aligned}$$

Then, we may calculate the time derivatives of the elements of $\hat{\rho}$:

$$\begin{aligned}
 \dot{\rho}_{ee} &= \langle e | \dot{\hat{\rho}} | e \rangle = -\gamma (\langle e | \hat{\sigma}_+ \hat{\sigma}_- \hat{\rho} | e \rangle + \langle e | \hat{\rho} \hat{\sigma}_+ \hat{\sigma}_- | e \rangle) \\
 &= -\gamma (\langle g | \hat{\sigma}_- \hat{\rho} | e \rangle + \langle e | \hat{\rho} \hat{\sigma}_+ | g \rangle) \\
 &= -\gamma (\langle e | \hat{\rho} | e \rangle + \langle e | \hat{\rho} | e \rangle) = -2\gamma \rho_{ee}.
 \end{aligned}$$

Analogously, we have for $\dot{\rho}_{gg}$:

$$\begin{aligned}
 \dot{\rho}_{gg} &= \langle g | \dot{\hat{\rho}} | g \rangle = \gamma (2\langle g | \hat{\sigma}_- \hat{\rho} \hat{\sigma}_+ | g \rangle - \langle g | \hat{\sigma}_+ \hat{\sigma}_- \hat{\rho} | g \rangle - \langle g | \hat{\rho} \hat{\sigma}_+ \hat{\sigma}_- | g \rangle) \\
 &= 2\gamma \langle e | \hat{\rho} | e \rangle = 2\gamma \rho_{ee}.
 \end{aligned}$$

For the time derivative of the matrix element ρ_{eg} , we have

$$\begin{aligned}\dot{\rho}_{eg} &= \left\langle e \left| \dot{\hat{\rho}} \right| g \right\rangle = \gamma \left(2 \left\langle e \left| \hat{\sigma}_- \hat{\rho} \hat{\sigma}_+ \right| g \right\rangle - \left\langle e \left| \hat{\sigma}_+ \hat{\sigma}_- \hat{\rho} \right| g \right\rangle - \left\langle e \left| \hat{\rho} \hat{\sigma}_+ \hat{\sigma}_- \right| g \right\rangle \right) \\ &= -\gamma \left\langle g \left| \hat{\sigma}_- \hat{\rho} \right| g \right\rangle = -\gamma \left\langle e \left| \hat{\rho} \right| g \right\rangle \\ &= -\gamma \rho_{eg}.\end{aligned}$$

The solutions of these differential equations are then given by

$$\begin{aligned}\rho_{ee}(t) &= e^{-2\gamma t} \rho_{ee}(0), \\ \rho_{gg}(t) &= 1 + e^{-2\gamma t} [\rho_{gg}(0) - 1], \\ \rho_{eg}(t) &= e^{-\gamma t} \rho_{eg}(0),\end{aligned}$$

where, for deriving the second solution, we have used the following procedure:

$$\begin{aligned}\rho_{gg}(t) &= 1 - \rho_{ee}(t) = 1 - e^{-2\gamma t} \rho_{ee}(0) \\ &= 1 - e^{-2\gamma t} [1 - \rho_{gg}(0)].\end{aligned}$$

From these results, it follows that the time derivatives of the Bloch vector's components are

$$\begin{aligned}\dot{s}_x &= \dot{\rho}_{eg} + \dot{\rho}_{ge} = -\gamma (\rho_{eg} + \rho_{ge}) = -\gamma s_x, \\ \dot{s}_y &= i (\dot{\rho}_{eg} - \dot{\rho}_{ge}) = -i\gamma (\rho_{eg} - \rho_{ge}) = -\gamma s_y, \\ \dot{s}_z &= \dot{\rho}_{ee} - \dot{\rho}_{gg} = -2\gamma \rho_{ee} - 2\gamma \rho_{ee} = -4\gamma \rho_{ee} = -2\gamma (1 + s_z).\end{aligned}$$

The solution of these differential equations are finally

$$\begin{aligned}s_x(t) &= e^{-\gamma t} s_x(0), \\ s_y(t) &= i e^{-\gamma t} [\rho_{eg}(0) - \rho_{ge}(0)] = e^{-\gamma t} s_y(0), \\ s_z(t) &= \rho_{ee}(t) - \rho_{gg}(t) = e^{-2\gamma t} \rho_{ee}(0) - 1 - e^{-2\gamma t} \rho_{gg}(0) + e^{-2\gamma t} \\ &= e^{-2\gamma t} s_z(0) + e^{-2\gamma t} - 1,\end{aligned}$$

which are in agreement with Eqs. (14.83).

14.10 This equation plays an important role and it can be proved in many ways. Let us call $L(\xi, \eta)$ the left-hand side and $R(\xi, \eta)$ the right-hand side.

A first possibility is to verify that:

- Both terms are equal to the identity at $\xi = 0$.
- Both terms satisfy the same differential equation

$$\frac{\partial L(\xi, \eta)}{\partial \xi} = (\hat{O} + \eta \hat{O}') L(\xi, \eta), \quad \frac{\partial R(\xi, \eta)}{\partial \xi} = (\hat{O} + \eta \hat{O}') R(\xi, \eta).$$

The proof of the first equation is trivial (it is essentially the definition of the exponential), while the proof of the second equation can be obtained by inspecting the different terms.

Both the functions $L(\xi, \eta)$ and $R(\xi, \eta)$ satisfy the same first-order differential equation with the same boundary condition and therefore they must be equal.

A second proof can be obtained by performing the following steps:

- One verifies that, for small ξ ,

$$R(\xi, \eta) = 1 + (\hat{O} + \eta \hat{O}')\xi + O(\xi^2).$$

- The function $R(\xi, \eta)$ satisfies the semigroup property (see Sec. 8.4)

$$R(\xi_1, \eta)R(\xi_2, \eta) = R(\xi_1 + \xi_2, \eta),$$

as can be proved by combining the different terms present in the lhs.

The function $L(\xi, \eta)$ trivially satisfies the same equations. The two properties identify in a unique way the function and therefore the two functions must coincide.

However the most instructive (and constructing) way to verify Eq. (14.91) is to check that the lhs and the rhs do coincide term by term in the Taylor expansion around $\eta = 0$. The Taylor expansion of the rhs is trivial, so we have to compute the Taylor expansion of the lhs. To this end it is convenient to notice that, for any real $\delta \neq 0$, we can write

$$L(\xi, \eta) = (e^{(\hat{O} + \eta \hat{O}')\delta})^{\frac{\xi}{\delta}}.$$

In particular, we can write

$$L(\xi, \eta) = \lim_{\delta \rightarrow 0} (e^{(\hat{O} + \eta \hat{O}')\delta})^{\frac{\xi}{\delta}} = \lim_{\delta \rightarrow 0} (1 + \delta(\hat{O} + \eta \hat{O}'))^{\frac{\xi}{\delta}}.$$

Without loss of generality we can evaluate the limit $\delta \rightarrow 0$ by restricting to the sequence of δ where $\zeta = \xi/\delta$ is an integer. Using this definition of ζ we have

$$L(\xi, \eta) = \lim_{\delta \rightarrow 0} \prod_{j=1, \zeta} (1 + \delta(\hat{O} + \eta \hat{O}')).$$

We can now easily compute the expansion in powers of η of the previous formula: the rhs is the product of terms linear in η . Let us compute the coefficient of the order η^2 . The term η^2 may come from both the j -th and the l -th terms of the product (where all the other factors give a contribution equal to $1/\delta \hat{O}$). We thus find that the coefficient of η^2 is just given by

$$\begin{aligned} \delta^2 \sum_{j,l=1,\zeta; j < l} & \left(\left(\prod_{a=1, j-1} (1 + \delta \hat{O}) \right) \hat{O}' \left(\prod_{b=j+1, l-1} (1 + \delta \hat{O}) \right) \hat{O}' \left(\prod_{c=l+1, \zeta} (1 + \delta \hat{O}) \right) \right) \\ & = \delta^2 \sum_{j,l=1,\zeta; j < l} (1 + \delta \hat{O})^{j-1} \hat{O}' (1 + \delta \hat{O})^{l-j-2} \hat{O}' (1 + \delta \hat{O})^{\zeta-l-1}. \end{aligned}$$

In the limit $\delta \rightarrow 0$ each individual term in the sum over j and l is irrelevant and we can assume that both j and l are of order δ^{-1} . We can thus substitute the sums with integrals; neglecting terms going to zero with δ we obtain

$$\int_0^\xi d\xi_1 \int_{\xi_1}^\xi d\xi_2 (1 + \delta \hat{O})^{\frac{\xi_1}{\delta}} \hat{O}' (1 + \delta \hat{O})^{\frac{\xi_2 - \xi_1}{\delta}} \hat{O}' (1 + \delta \hat{O})^{\frac{\xi - \xi_2}{\delta}}.$$

We can now perform the limit $\delta \rightarrow 0$ and obtain

$$\int_0^\xi d\xi_1 \int_{\xi_1}^\xi d\xi_2 e^{\xi_1 \hat{O}} \hat{O}' e^{(\xi_2 - \xi_1) \hat{O}} \hat{O}' e^{(\xi - \xi_2) \hat{O}},$$

which is essential the result stated in Eq. (14.91) for $k = 2$, apart from a redefinition of the integration variables. It should be clear to the reader how to generalize the result to higher (and lower) values of k .

The same result could also be obtained starting from path integral representation (see Sec. 10.8) for the function $L(\xi, \eta)$, but we shall not show this further derivation. We should note that all the proofs presented here have a rather formal character: we are implicitly assuming that the rhs of Eq. (14.91) is a convergent series (and that the lhs exists). If not (the perturbative expansion is often not convergent), the rhs should be interpreted as an asymptotic expansion (see also Secs. 10.1–10.2).

14.11 Let us start from the identity

$$\hat{\rho} = |\psi\rangle\langle\psi|.$$

Time derivation leads to

$$\dot{\hat{\rho}} = |\dot{\psi}\rangle\langle\psi| + |\psi\rangle\langle\dot{\psi}|,$$

where

$$|\dot{\psi}\rangle = \frac{1}{i\hbar} \tilde{H} |\psi\rangle, \quad \langle\dot{\psi}| = \frac{1}{\hbar} \langle\psi| \tilde{H}^\dagger.$$

Then, we have

$$\begin{aligned} \dot{\hat{\rho}} &= \frac{1}{i\hbar} \tilde{H} \hat{\rho} - \frac{1}{i\hbar} \hat{\rho} \tilde{H}^\dagger \\ &= \frac{1}{i\hbar} (\hat{H}_0 + \hat{H}') \hat{\rho} - \frac{1}{i\hbar} \hat{\rho} (\hat{H}_0 + \hat{H}') \\ &= \frac{1}{i\hbar} [\hat{H}_0, \hat{\rho}] + \frac{1}{i\hbar} [\hat{H}', \hat{\rho}]_+. \end{aligned}$$

14.13 First, the reader may verify that the exponential $e^{-\iota \frac{\pi}{2} t j^2}$ is equal to 1 for even values of j ($j = 2k$) and to $-\iota$ for odd values of j ($j = 2k + 1$). Then, we have

$$\begin{aligned} e^{-\frac{|\alpha|^2}{2}} \sum_{j=0}^{\infty} \alpha^j \frac{e^{-\iota \frac{\pi}{2} t j^2}}{\sqrt{j!}} |j\rangle &= \frac{e^{-\frac{|\alpha|^2}{2}}}{2} \left[\sum_{k=0}^{\infty} \frac{2\alpha^{2k}}{\sqrt{2k!}} |2k\rangle + \sum_{k=0}^{\infty} (-2\iota) \frac{\alpha^{2k+1}}{\sqrt{(2k+1)!}} |2k+1\rangle \right] \\ &= e^{-\frac{|\alpha|^2}{2}} \left[(1 + \iota) \sum_{k=0}^{\infty} \frac{\alpha^{2k}}{\sqrt{2k!}} |2k\rangle + (1 - \iota) \sum_{k=0}^{\infty} \frac{\alpha^{2k}}{\sqrt{(2k)!}} |2k\rangle \right. \\ &\quad \left. + (1 - \iota) \sum_{k=0}^{\infty} \frac{\alpha^{2k+1}}{\sqrt{(2k+1)!}} |2k+1\rangle - (1 + \iota) \sum_{k=0}^{\infty} \frac{\alpha^{2k+1}}{\sqrt{(2k+1)!}} |2k+1\rangle \right], \end{aligned}$$

where we have made use of the identities $2 = 1 + \iota + 1 - \iota$ and $-2\iota = 1 - \iota - (1 + \iota)$. Now we group the first and last terms, and the second and third terms of the rhs, so as to obtain

$$\begin{aligned}
e^{-\frac{|\alpha|^2}{2}} \sum_{j=0}^{\infty} \alpha^j \frac{e^{-\frac{\pi}{2} t j^2}}{\sqrt{j!}} |j\rangle &= \frac{1}{\sqrt{2}} \left[\frac{(1-\iota)}{\sqrt{2}} e^{-\frac{|\alpha|^2}{2}} \sum_{k=0}^{\infty} \frac{\alpha^k}{\sqrt{k!}} |k\rangle + \frac{(1+\iota)}{\sqrt{2}} e^{-\frac{|\alpha|^2}{2}} \right. \\
&\quad \left. \sum_{k=0}^{\infty} \frac{(-\alpha)^k}{\sqrt{k!}} |k\rangle \right] \\
&= \frac{1}{\sqrt{2}} \left(e^{-\iota \frac{\pi}{4}} |\alpha\rangle + e^{\iota \frac{\pi}{4}} |-\alpha\rangle \right),
\end{aligned}$$

where we have made use of the mathematical identity

$$\frac{(1 \pm \iota)}{\sqrt{2}} = e^{\pm \iota \frac{\pi}{4}}$$

and of the fact that (see Eq. (13.58))

$$e^{-\frac{|\alpha|^2}{2}} \sum_{k=0}^{\infty} \frac{(\pm\alpha)^k}{\sqrt{k!}} |k\rangle = |\pm\alpha\rangle.$$

14.15 Any distance between two elements a, b has to satisfy four well-known properties. The property $d(a, a) = 0$ is easily satisfied by the Fubini–Study distance, since $|\langle\psi_1 | \psi_1\rangle|^2 = 1$. Similarly, the Fubini–Study distance is always positive when the two states are different except the trivial case in which the difference is only given by the global phase, since $|\langle\psi_1 | \psi_2\rangle|^2 < 1$. Also the property that $d(a, b) = d(b, a)$, since $|\langle\psi_1 | \psi_2\rangle|^2 = |\langle\psi_2 | \psi_1\rangle|^2$. Finally, the triangular property $d(a, b) + d(b, c) \geq d(a, c)$ is also satisfied. Indeed we have

$$\sqrt{1 - |\langle\psi_1 | \psi_2\rangle|^2} + \sqrt{1 - |\langle\psi_2 | \psi_3\rangle|^2} \geq \sqrt{1 - |\langle\psi_1 | \psi_3\rangle|^2}.$$

To prove this, it suffices to assume, without loss of generality, that the involved state vectors are normalized and real. Then, consider that

$$||\psi_1\rangle - |\psi_2\rangle|^2 = 2 - 2\langle\psi_1 | \psi_2\rangle,$$

from which it follows that it suffices to multiply both the lhs and the rhs of the above inequality so as to obtain

$$||\psi_1\rangle - |\psi_2\rangle| + ||\psi_2\rangle - |\psi_3\rangle| \geq ||\psi_1\rangle - |\psi_3\rangle|,$$

which is satisfied, since it is an instance of the triangular inequality (see also Subsec. 2.3.2)

$$|a| + |b| \geq |a + b|.$$

When applying the definition of the Fubini–Study distance to the distance between the coherent states in Box 14.1, we must make use of the square modulus (Eq. (13.70)), so that

$$d_{fs} = \sqrt{1 - e^{-|\alpha e^{i\phi} - \alpha e^{-i\phi}|^2}} = \sqrt{1 - e^{-4|\alpha|^2 \sin^2 \phi}}.$$

Expanding in power series to the first-order in $\sin \phi$ for $\phi \ll 1$, we obtain

$$d_{fs} \simeq 2|\alpha| \sin \phi = d.$$

Chapter 15

15.1 If you do not succeed, please refer to the quoted specialized literature.

15.7 It is easy to prove that (see also Prob. 13.21)

$$\begin{aligned}\hat{\Pi}_{xp}\hat{D}_{xp}|\psi^n\rangle &= \hat{D}_{xp}\hat{\Pi}\hat{D}_{xp}^{-1}|\psi^n\rangle \\ &= \hat{D}_{xp}\hat{\Pi}|\psi^n\rangle \\ &= \hat{D}_{xp}(-1)^n|\psi^n\rangle \\ &= (-1)^n|\psi_{xp}^n\rangle,\end{aligned}$$

from which the solution follows.

15.9 First of all, we note that the exponential factor $e^{-\xi\alpha^*+\xi^*\alpha}$ may be rewritten as $e^{2i(\xi_r\alpha_i-\xi_i\alpha_r)}$. We start from Eq. (15.59), which then turns to

$$W(\alpha_r, \alpha_i) = \frac{1}{\pi^2} \int_{-\infty}^{+\infty} d\xi_r d\xi_i e^{2i(\xi_r\alpha_i-\xi_i\alpha_r)} \chi(\xi_r, \xi_i).$$

Changing the variables according to

$$\xi_r = -\frac{1}{\sqrt{2}}\zeta \sin \theta \quad \text{and} \quad \xi_i = \frac{1}{\sqrt{2}}\zeta \cos \theta,$$

we also have $d\xi_r d\xi_i = \frac{1}{2}|\zeta| d\zeta d\theta$, and, using Eq. (15.64), we may rewrite the W-function as

$$W(\alpha_r, \alpha_i) = \frac{1}{2\pi^2} \int_{-\infty}^{+\infty} d\zeta \int_0^\pi d\theta |\zeta| e^{-i\sqrt{2}\zeta(\alpha_i \sin \theta + \alpha_r \cos \theta)} \chi_\wp(\zeta, \theta).$$

Making the inverse Fourier transform of Eq. (15.61), that is,

$$\chi_\wp(\zeta, \theta) = \int dX \wp(X, \theta) e^{i\zeta X},$$

and inserting this into the previous equation, we finally obtain

$$W(\alpha_r, \alpha_i) = \frac{1}{2\pi^2} \int_{-\infty}^{+\infty} dX \int_{-\infty}^{+\infty} d\zeta \int_0^\pi d\theta |\zeta| \wp(X, \theta) e^{i\zeta[X - \sqrt{2}(\alpha_r \cos \theta + \alpha_i \sin \theta)]}.$$

15.11 We sketch the main steps of the derivation. First, since all the basis states in Eq. (15.71) are orthogonal, perform the square modulus of Eq. (15.72), so as to obtain (see Sec. 9.9)

$$\wp_e(t, \phi) = \sum_{n=0}^{\infty} |\psi_{e,n}(t)|^2.$$

Then, make use of the following facts:

$$\begin{aligned}\sum_{n=0}^{\infty} |c_{n+1}|^2 &= 1 - |c_0|^2, \\ \imath(z - z^*) &= -2\Im(z), \quad z \in \mathbb{C}, \\ 2 \sin \theta \cos \theta &= \sin 2\theta, \\ \cos^2 \theta &= \frac{1 + \cos 2\theta}{2}.\end{aligned}$$

Chapter 16

16.1 From Eqs. (16.3)–(16.5) we have

$$\begin{aligned}\Psi(x_1, x_2) &= \frac{1}{2\pi} \int_{-\infty}^{+\infty} dp e^{\frac{i}{\hbar}(x_1 - x_2 + x_0)p} \\ &= \frac{\hbar}{\sqrt{2\pi}} \delta(x_1 - x_2 + x_0) = \frac{\hbar}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dx \delta(x_1 - x) \delta(x - x_2 + x_0) \\ &= \frac{1}{2\pi} \int_{-\infty}^{+\infty} dx \delta(x_1 - x) \int_{-\infty}^{+\infty} dp e^{-\frac{i}{\hbar}(x - x_2 + x_0)p} \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dx \psi_x(x_2) \varphi_x(x_1).\end{aligned}$$

16.4 Let us take $|\varsigma\rangle = |\varsigma_k\rangle$ as an element of a complete set of orthogonal vectors $\{|\varsigma_j\rangle\}$.

Then, by Eq. (16.27), and by the fact that each $\langle \hat{P}_{\varsigma_j} \rangle_{\varphi}$ cannot be negative, we immediately have that for any $j \neq k$ all $\langle \hat{P}_{\varsigma_j} \rangle_{\varphi}$ vanish.

16.6 Since $\langle \hat{P}_{\varsigma_1} \rangle_{\varphi} = \langle \hat{P}_{\varsigma_2} \rangle_{\varphi} = 0$, then the rhs of Eq. (16.29) vanishes, which in turn implies that $\langle \hat{P}_{\psi_1} \rangle_{\varphi} = \langle \hat{P}_{\psi_2} \rangle_{\varphi} = 0$. Writing, e.g., $|\psi_1\rangle$ as the linear combination

$$|\psi_1\rangle = c_1 |\varsigma_1\rangle + c_2 |\varsigma_2\rangle,$$

with arbitrary c_1, c_2 , we obtain the desired result.

16.8 The problem is solved when considering that (see Eqs. (6.154))

$$\begin{aligned}\hat{\sigma}_1 \cdot \mathbf{a} &= a_x \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}_1 + a_y \begin{bmatrix} 0 & -\imath \\ \imath & 0 \end{bmatrix}_1 + a_z \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}_1 \\ \text{and} \\ \hat{\sigma}_2 \cdot \mathbf{b} &= b_x \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}_2 + b_y \begin{bmatrix} 0 & -\imath \\ \imath & 0 \end{bmatrix}_2 + b_z \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}_2,\end{aligned}$$

The expectation value on the singlet state (16.12) of the product of these two scalar products gives nine terms, of which the first three have the form

$$\begin{aligned}
\langle \Psi_0 | a_x b_x \hat{\sigma}_{1x} \hat{\sigma}_{2x} | \Psi_0 \rangle &= \langle \Psi_0 | \frac{a_x b_x}{\sqrt{2}} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}_1 \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}_2 \\
&\quad \times \left[\begin{pmatrix} 1 \\ 0 \end{pmatrix}_1 \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix}_2 - \begin{pmatrix} 0 \\ 1 \end{pmatrix}_1 \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix}_2 \right] \\
&= \langle \Psi_0 | \frac{a_x b_x}{\sqrt{2}} \left[\begin{pmatrix} 0 \\ 1 \end{pmatrix}_1 \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix}_2 - \begin{pmatrix} 1 \\ 0 \end{pmatrix}_1 \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix}_2 \right] \\
&= \langle \Psi_0 | -a_x b_x | \Psi_0 \rangle = -a_x b_x.
\end{aligned}$$

Similar calculations show that we also have

$$\langle \Psi_0 | a_y b_y \hat{\sigma}_{1y} \hat{\sigma}_{2y} | \Psi_0 \rangle = -a_y b_y \quad \text{and} \quad \langle \Psi_0 | a_z b_z \hat{\sigma}_{1z} \hat{\sigma}_{2z} | \Psi_0 \rangle = -a_z b_z.$$

The six cross terms are instead all zero. Indeed, we have

$$\begin{aligned}
\langle \Psi_0 | a_x b_y \hat{\sigma}_{1x} \hat{\sigma}_{2y} | \Psi_0 \rangle &= \langle \Psi_0 | \frac{a_x b_y}{\sqrt{2}} \left[\begin{pmatrix} 0 \\ 1 \end{pmatrix}_1 \otimes \begin{pmatrix} -i \\ 0 \end{pmatrix}_2 - \begin{pmatrix} 1 \\ 0 \end{pmatrix}_1 \otimes \begin{pmatrix} 0 \\ i \end{pmatrix}_2 \right] \\
&= \frac{a_x b_y}{2} \left[(1 \ 0)_1 \otimes (0 \ 1)_2 - (0 \ 1)_1 \otimes (1 \ 0)_2 \right] \\
&\quad \times \left[\begin{pmatrix} 0 \\ 1 \end{pmatrix}_1 \otimes \begin{pmatrix} -i \\ 0 \end{pmatrix}_2 - \begin{pmatrix} 1 \\ 0 \end{pmatrix}_1 \otimes \begin{pmatrix} 0 \\ i \end{pmatrix}_2 \right] \\
&= \frac{a_x b_y}{2} [-(1 \cdot i) - (1 \cdot (-i))] = 0,
\end{aligned}$$

and similarly for all other cross terms, so that we may finally conclude that

$$\langle \Psi_0 | (\hat{\sigma}_1 \cdot \mathbf{a}) (\hat{\sigma}_2 \cdot \mathbf{b}) | \Psi_0 \rangle = -(a_x b_x + a_y b_y + a_z b_z) = -\mathbf{a} \cdot \mathbf{b}.$$

16.9 The solution is obtained when one considers that, for any integrable function $f(x)$, we have

$$\left| \int dx f(x) \right| \leq \int dx |f(x)|,$$

and $|A_{\mathbf{b}}(\lambda)A_{\mathbf{c}}(\lambda) - 1| = 1 - A_{\mathbf{b}}(\lambda)A_{\mathbf{c}}(\lambda)$

16.10 We have that

$$\begin{aligned}
\langle \mathbf{a}', \mathbf{b} \rangle &= \int_{\Lambda} d\lambda \rho(\lambda) A_{\mathbf{a}'}(\lambda) B_{\mathbf{b}}(\lambda) = 1 - \delta \\
&= \int_{\Lambda^+} d\lambda \rho(\lambda) - \int_{\Lambda^-} d\lambda \rho(\lambda).
\end{aligned}$$

Since

$$\int_{\Lambda^+} d\lambda \rho(\lambda) + \int_{\Lambda^-} d\lambda \rho(\lambda) = 1,$$

we immediately obtain the desired result.

16.11 Making use of Eq. (16.65), we have that

$$\int_{\Lambda} d\lambda \rho(\lambda) B_{\mathbf{b}}(\lambda) B_{\mathbf{b}'}(\lambda) = \int_{\Lambda^+} d\lambda \rho(\lambda) A_{\mathbf{a}'}(\lambda) B_{\mathbf{b}'}(\lambda) - \int_{\Lambda^-} d\lambda \rho(\lambda) A_{\mathbf{a}'}(\lambda) B_{\mathbf{b}'}(\lambda),$$

which together with the fact that

$$\int_{\Lambda^+} d\lambda \rho(\lambda) B_{\mathbf{b}}(\lambda) B_{\mathbf{b}'}(\lambda) = \int_{\Lambda} d\lambda \rho(\lambda) A_{\mathbf{a}'}(\lambda) B_{\mathbf{b}'}(\lambda) - \int_{\Lambda^-} d\lambda \rho(\lambda) A_{\mathbf{a}'}(\lambda) B_{\mathbf{b}'}(\lambda),$$

allows us to derive

$$\int_{\Lambda} d\lambda \rho(\lambda) B_{\mathbf{b}}(\lambda) B_{\mathbf{b}'}(\lambda) = \int_{\Lambda} d\lambda \rho(\lambda) A_{\mathbf{a}'}(\lambda) B_{\mathbf{b}'}(\lambda) - 2 \int_{\Lambda^-} d\lambda \rho(\lambda) A_{\mathbf{a}'}(\lambda) B_{\mathbf{b}'}(\lambda).$$

Now, we also have that

$$\begin{aligned} & \int_{\Lambda} d\lambda \rho(\lambda) A_{\mathbf{a}'}(\lambda) B_{\mathbf{b}'}(\lambda) - 2 \int_{\Lambda^-} d\lambda \rho(\lambda) A_{\mathbf{a}'}(\lambda) B_{\mathbf{b}'}(\lambda) \\ & \geq \int_{\Lambda} d\lambda \rho(\lambda) A_{\mathbf{a}'}(\lambda) B_{\mathbf{b}'}(\lambda) - 2 \int_{\Lambda^-} d\lambda \rho(\lambda) |A_{\mathbf{a}'}(\lambda) B_{\mathbf{b}'}(\lambda)|. \end{aligned}$$

Since $A_{\mathbf{a}'}(\lambda) B_{\mathbf{b}'}(\lambda) = \pm 1$, these results, together with Eqs. (16.66) and (16.62), give the desired solution.

16.12 Let us do the substitution $\mathbf{a}' = \mathbf{b}'$ in inequality (16.69) in its formulation:

$$|\langle \mathbf{a}, \mathbf{b} \rangle - \langle \mathbf{a}, \mathbf{b}' \rangle| \leq 2 + \langle \mathbf{a}', \mathbf{b}' \rangle + \langle \mathbf{a}', \mathbf{b} \rangle.$$

Since

$$\langle \mathbf{b}', \mathbf{b}' \rangle = -1,$$

the result is easily obtained.

16.13 By making use of Eq. (16.53), let us first rewrite Eq. (16.55) as

$$\begin{aligned} \langle \mathbf{a}, \mathbf{b} \rangle - \langle \mathbf{a}, \mathbf{b}' \rangle &= \int d\lambda \rho(\lambda) [A_{\mathbf{a}}(\lambda) B_{\mathbf{b}}(\lambda) (1 \pm A_{\mathbf{a}'}(\lambda) B_{\mathbf{b}'}(\lambda))] \\ &\quad - \int d\lambda \rho(\lambda) [A_{\mathbf{a}}(\lambda) B_{\mathbf{b}'}(\lambda) (1 \pm A_{\mathbf{a}'}(\lambda) B_{\mathbf{b}}(\lambda))]. \end{aligned}$$

Since we have that

$$[A_{\mathbf{a}}(\lambda)]^2 = 1 \geq A_{\mathbf{a}}(\lambda) B_{\mathbf{b}}(\lambda), \quad A_{\mathbf{a}}(\lambda) B_{\mathbf{b}'}(\lambda),$$

which implies both

$$\begin{aligned} \int d\lambda \rho(\lambda) [A_{\mathbf{a}}(\lambda) B_{\mathbf{b}}(\lambda) (1 \pm A_{\mathbf{a}'}(\lambda) B_{\mathbf{b}'}(\lambda))] &\leq \int d\lambda \rho(\lambda) (1 \pm A_{\mathbf{a}'}(\lambda) B_{\mathbf{b}'}(\lambda)) \\ \int d\lambda \rho(\lambda) [A_{\mathbf{a}}(\lambda) B_{\mathbf{b}'}(\lambda) (1 \pm A_{\mathbf{a}'}(\lambda) B_{\mathbf{b}}(\lambda))] &\leq \int d\lambda \rho(\lambda) (1 \pm A_{\mathbf{a}'}(\lambda) B_{\mathbf{b}}(\lambda)), \end{aligned}$$

we also have

$$|\langle \mathbf{a}, \mathbf{b} \rangle - \langle \mathbf{a}, \mathbf{b}' \rangle| \leq \int d\lambda \rho(\lambda) (1 \pm A_{\mathbf{a}'}(\lambda) B_{\mathbf{b}'}(\lambda)) + \int d\lambda \rho(\lambda) (1 \pm A_{\mathbf{a}'}(\lambda) B_{\mathbf{b}}(\lambda)),$$

which amounts to

$$|\langle \mathbf{a}, \mathbf{b} \rangle - \langle \mathbf{a}, \mathbf{b}' \rangle| \leq 2 \pm \langle \mathbf{a}', \mathbf{b}' \rangle \pm \langle \mathbf{a}', \mathbf{b} \rangle,$$

from which the CHSH inequality follows.

16.14 From Eqs. (16.73), (16.75), and (16.172) we obtain

$$\begin{aligned} -1 \leq \pi_{12}(\lambda, \mathbf{a}, \mathbf{b}) - \pi_{12}(\lambda, \mathbf{a}, \mathbf{b}') + \pi_{12}(\lambda, \mathbf{a}', \mathbf{b}) + \pi_{12}(\lambda, \mathbf{a}', \mathbf{b}') \\ - \pi_1(\lambda, \mathbf{a}') - \pi_2(\lambda, \mathbf{b}) \leq 0, \end{aligned}$$

where in Eqs. (16.171) we have taken

$$\begin{aligned} x_k &= \pi_k(\lambda, \mathbf{j}), \quad \text{with } \mathbf{j} = \{\mathbf{a}, \mathbf{a}'\}, \\ y_k &= \pi_k(\lambda, \mathbf{l}), \quad \text{with } \mathbf{l} = \{\mathbf{b}, \mathbf{b}'\}, \end{aligned}$$

and $X = Y = 1$. Integrating this inequality over Λ with the probability distribution ρ_λ , and using Eqs. (16.74), yields

$$-1 \leq \wp_{12}(\mathbf{a}, \mathbf{b}) - \wp_{12}(\mathbf{a}, \mathbf{b}') + \wp_{12}(\mathbf{a}', \mathbf{b}) + \wp_{12}(\mathbf{a}', \mathbf{b}') - \wp_1(\mathbf{a}') - \wp_2(\mathbf{b}) \leq 0,$$

which may be rewritten as Eq. (16.76).

16.19 The three-particle interference in the GHSZ state (Eq. (16.143)) is evidenced by the sine term in Eq. (16.144a), which represents the probability that the three particles are detected at D1, D2, and D3. In order to test if the two-particle interference is present, we have to consider the probability that two detectors (say D2 and D3) click independently of what happens in the third arm of the inteferometer. In this case, for instance, we have to sum Eqs. (16.144a) and (16.144b) and obtain $\wp_{D_2 D_3}^\Psi(\phi_1, \phi_2, \phi_3) = 1/4$, which is independent of the phases ϕ_1, ϕ_2 , and ϕ_3 .

Chapter 17

17.2 In the case of pure states, we have $\hat{\rho} = \hat{P}_k = |b_k\rangle \langle b_k|$, which means that in Eq. (17.4) we have $w_k \delta_{jk}$, with the consequence that the diagonal matrix has only an element different from zero, namely $w_k = 1$. This proves the result because the logarithmic function of 1 is 0.

17.8 Applying one of the unitary operators (17.73) to the corresponding state of particle 3 as represented in Eq. (17.71), we recover the information contained in particle 1, which may be rewritten in the form

$$c \begin{pmatrix} 1 \\ 0 \end{pmatrix}_1 + c' \begin{pmatrix} 0 \\ 1 \end{pmatrix}_1 = \begin{pmatrix} c \\ c' \end{pmatrix}_1.$$

Indeed,

$$\left\{ \begin{array}{l} \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix}_3 \begin{pmatrix} -c \\ -c' \end{pmatrix}_3 \\ \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}_3 \begin{pmatrix} -c \\ c' \end{pmatrix}_3 \\ \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}_3 \begin{pmatrix} c' \\ c \end{pmatrix}_3 \\ \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}_3 \begin{pmatrix} -c' \\ c \end{pmatrix}_3 \end{array} \right\} = \begin{pmatrix} c \\ c' \end{pmatrix}_3.$$

In the case of the first measurement outcome (the singlet one), the state of particle 3 is the same as of particle 1 except for an irrelevant phase factor, so that Bob need do nothing further to reproduce the state of 1. In the three other cases, Bob must apply one of the unitary operators $\hat{U}_2, \hat{U}_3, \hat{U}_4$ – corresponding, respectively, to 180° rotations around the z -, x -, y -axes – in order to convert the state of 3 into the state of 1. What Bob must do, obviously depends on the (classical) communication of Alice's result.

- 17.10** The most direct algorithm that can be used to factorize an integer number of l digits consists of checking whether the integer is divisible by each number from 2 to $\sqrt{M} = \sqrt{10^l}$. Therefore, this algorithm requires a number of steps given by

$$N \simeq \sqrt{M} = \sqrt{10^l},$$

which shows that the growth is exponential. For example, if l is equal to 100 decimal digits, even if the time required for a division is very small (say, 10^{-20} s), the total time required to factorize the original number is

$$\tau \simeq 10^{10} \times 10^{-20} = 10^{30} \text{ s},$$

i.e. 10^{13} times the age of the universe. Of course, in the example above we have not chosen the most efficient algorithm. As a matter of fact, the best known classical algorithm takes a time of the order of $10^{l^{1/3}}$ (i.e. it is sub-exponential).

- 17.11** The state (17.109) on which we want to evaluate the Boolean function may be rewritten as

$$\frac{1}{2} (|0\rangle + |1\rangle) (|0\rangle - |1\rangle) = \frac{1}{2} (|00\rangle - |01\rangle + |10\rangle - |11\rangle).$$

Now, we evaluate each of the four components of the state above for each of the four possible Boolean functions f_j ($j = 1, \dots, 4$), i.e.

$$\begin{aligned} f_1 : |00\rangle - |01\rangle + |10\rangle - |11\rangle &= (|0\rangle \hat{E} + |1\rangle) (|0\rangle - |1\rangle), \\ f_2 : |01\rangle - |00\rangle + |11\rangle - |10\rangle &= (|0\rangle \hat{E} + |1\rangle) (|1\rangle - |0\rangle), \\ f_3 : |00\rangle - |01\rangle + |11\rangle - |10\rangle &= (|0\rangle \hat{E} - |1\rangle) (|0\rangle - |1\rangle), \\ f_4 : |01\rangle - |00\rangle + |10\rangle - |11\rangle &= (|0\rangle \hat{E} - |1\rangle) (|1\rangle - |0\rangle). \end{aligned}$$

This leads to the desired solution.

- 17.12** The distance between $\hat{\rho}_1$ and $\hat{\rho}_2$ is given by

$$\begin{aligned} d(\hat{\rho}_1, \hat{\rho}_2) &= \frac{1}{2} \text{Tr} |\hat{\rho}_1 - \hat{\rho}_2| \\ &= \frac{1}{4} \text{Tr} |(\mathbf{r} - \mathbf{s}) \cdot \hat{\sigma}| \\ &= \frac{1}{2} |\mathbf{r} - \mathbf{s}|, \end{aligned}$$

since $(\mathbf{r} - \mathbf{s}) \cdot \hat{\sigma}$ has eigenvalues $\pm |\mathbf{r} - \mathbf{s}|$, so that we obtain

$$\text{Tr} |(\mathbf{r} - \mathbf{s}) \cdot \hat{\sigma}| = 2 |\mathbf{r} - \mathbf{s}|.$$

In other words, we have the important result that the distance between two single qubit states is equal to one half the Euclidean distance between them on the Bloch sphere. Since rotation on the Bloch sphere leaves this distance unaffected, unitary transformations preserve it, i.e.

$$d(\hat{\rho}_1, \hat{\rho}_2) = d(\hat{U} \hat{\rho}_1 \hat{U}^\dagger, \hat{U} \hat{\rho}_2 \hat{U}^\dagger).$$