

# Chapter 3

## The Heisenberg Realization of Quantum Mechanics

In this chapter, we present the simplest realization of the basic principles of quantum mechanics. We employ column vectors as state vectors and square matrices as operators. This formulation is especially suitable for Hilbert spaces with finite dimensions. However, we also treat within this framework the problem of the harmonic oscillator and the Jaynes–Cummings model.

### 3.1 Matrix Formalism

#### 3.1.1 A Realization of the Hilbert Space

The state vector  $\Psi$  may be expressed by means of the amplitudes  $c_i$  filling the successive rows of a column vector:

$$\Psi = (c_i) \equiv \begin{pmatrix} c_a \\ c_b \\ \vdots \\ c_v \end{pmatrix}. \quad (3.1)$$

The dimension of the Hilbert space is given by the number of rows. The sum of two column vectors is another column vector in which the amplitudes are added:

$$\alpha_B \Psi_B + \alpha_C \Psi_C = (\alpha_B b_i + \alpha_C c_i). \quad (3.2)$$

The scalar product requires the definition of the adjoint vector  $\Psi^+$ , i.e. a row vector obtained from  $\Psi$  with amplitudes

$$\Psi^+ = (c_a^*, c_b^*, \dots, c_v^*). \quad (3.3)$$

The scalar product of two vectors  $\Psi_B$  and  $\Psi_C$  is defined as the product of the adjoint vector  $\Psi_B^+$  and the vector  $\Psi_C$ , viz.,

$$\langle \Psi_B | \Psi_C \rangle = \sum_{i=a}^{i=v} b_i^* c_i,$$

$$\langle \Psi | \Psi \rangle = \sum_{i=a}^{i=v} |c_i|^2 = 1. \quad (3.4)$$

A useful set of (orthonormal) basis states is given by the vector columns  $\varphi_i$  with amplitudes  $c_j = \delta_{ij}$ . In such a basis, the arbitrary vector (3.1) may be expanded as

$$\Psi = c_a \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} + c_b \begin{pmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix} + \cdots + c_v \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix}. \quad (3.5)$$

All the properties listed in Table 2.1 are reproduced within the framework of column vectors.

Operators are represented by square matrices

$$\hat{Q} = (\langle i | Q | j \rangle) \equiv \begin{pmatrix} \langle a | Q | a \rangle & \langle a | Q | b \rangle & \cdots & \langle a | Q | v \rangle \\ \langle b | Q | a \rangle & \langle b | Q | b \rangle & \cdots & \langle b | Q | v \rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle v | Q | a \rangle & \langle v | Q | b \rangle & \cdots & \langle v | Q | v \rangle \end{pmatrix}. \quad (3.6)$$

The matrices corresponding to physical observables are Hermitian [see (2.11)]. The initial state  $j$  labels the columns, while the final state  $i$  labels the rows. The order  $a, b, \dots, v$  is immaterial, provided it is the same in both columns and rows (i.e. the matrix elements  $\langle i | Q | i \rangle$  should lie on the diagonal). The matrix elements  $\langle i | Q | j \rangle$  are constructed as in (2.10). If  $\varphi_i$  belongs to the basic set

$$\hat{Q} \varphi_i = \sum_j c_j^{(i)} \varphi_j \rightarrow \langle j | Q | i \rangle = c_j^{(i)}. \quad (3.7)$$

A matrix multiplying a vector yields another vector, so that

$$\Psi_B = \hat{Q} \Psi_C \longleftrightarrow b_i = \sum_j \langle i | Q | j \rangle c_j. \quad (3.8)$$

The product of two matrices is another matrix:

$$\hat{S} = \hat{Q} \hat{R} \longleftrightarrow \langle i|S|j\rangle = \sum_k \langle i|Q|k\rangle \langle k|R|j\rangle, \quad (3.9)$$

which is consistent with the closure property (2.59). The multiplication of matrices is a non-commutative operation, as befits the representation of quantum operators.

### 3.1.2 Solution of the Eigenvalue Equation

In matrix form, the eigenvalue equation (2.9) reads

$$\begin{pmatrix} \langle a|Q|a\rangle & \langle a|Q|b\rangle & \cdots & \langle a|Q|v\rangle \\ \langle b|Q|a\rangle & \langle b|Q|b\rangle & \cdots & \langle b|Q|v\rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle v|Q|a\rangle & \langle v|Q|b\rangle & \cdots & \langle v|Q|v\rangle \end{pmatrix} \begin{pmatrix} c_a \\ c_b \\ \vdots \\ c_v \end{pmatrix} = q \begin{pmatrix} c_a \\ c_b \\ \vdots \\ c_v \end{pmatrix}, \quad (3.10)$$

which is equivalent to the  $v$  linear equations (one equation for each value of  $i$ )

$$\sum_{j=1}^{j=v} \langle i|Q|j\rangle c_j = q c_i. \quad (3.11)$$

The eigenvalues  $q$  and the amplitudes  $c_i$  are the unknowns to be determined.<sup>1</sup>

The solution to (3.11) is obtained by casting the original matrix ( $\langle i|Q|j\rangle$ ) into a diagonal form. In this case the diagonal matrix elements become the eigenvalues,  $\langle i|Q|j\rangle = \delta_{ij} q_i$ . The  $i$ th eigenvector is given by the amplitudes  $c_j = \delta_{ij}$ , as in (3.5). For instance,

$$\begin{pmatrix} q_1 & 0 & \cdots & 0 \\ 0 & q_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & q_v \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix} = q_2 \begin{pmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix}. \quad (3.12)$$

The linear homogeneous equations (3.11) have the trivial solution  $c_i = 0$ , to be discarded. The existence of additional, non-trivial solutions requires the determinant to vanish:

$$\det(\langle i|Q|j\rangle - q\delta_{ij}) = 0. \quad (3.13)$$

<sup>1</sup>This equation may be obtained directly by using the expansion (2.6) on both sides of the general eigenvalue equation  $\hat{Q}\Psi = q\Psi$ . One obtains  $\sum_j c_j \hat{Q}\phi_j = q \sum_j c_j \phi_j$ . The scalar product with  $\phi_i$  of both sides of this last equation yields (3.11).

This eigenvalue equation is equivalent to a polynomial equation for  $q$ . Its  $\nu$  roots are the eigenvalues of the operator  $\hat{Q}$ .

The vanishing of the determinant (3.13) implies that one of the equations (3.11) may be expressed as a linear combination of the other  $\nu - 1$  equations. Therefore, by disregarding one of these equations (for instance, the one corresponding to the last row) and dividing the remaining equations by  $c_a$ , one obtains a set of  $\nu - 1$  non-homogeneous linear equations<sup>2</sup> yielding the value of the ratios  $c_b/c_a, c_c/c_a, \dots, c_\nu/c_a$ , for each eigenvalue  $q$ . The normalization equation (3.4) determines the value of  $|c_a|^2$ , up to the usual overall arbitrary phase of the state vector. Note that the relative phases in the linear combination have physical significance, although the overall phase is unimportant.

Diagonalization yields a new set of eigenstates  $\phi_a$ . Each of them may be expressed as a linear combination of the old basis states  $\varphi_i$ .

$$\phi_a = \sum_i \langle i|a \rangle \varphi_i. \quad (3.14)$$

The amplitudes  $\langle i|a \rangle$  are the matrix elements of a unitary matrix  $\mathcal{U} = (\langle i|a \rangle)$  (2.14). The modulus squared  $|\langle a|i \rangle|^2$  is both the probability of measuring the eigenvalue  $q_i$ , associated with the eigenstate  $\varphi_i$ , if the system is in the state  $\phi_a$ , and the probability of measuring the eigenvalue  $r_a$ , associated with the eigenstate  $\phi_a$ , when the state of the system is  $\varphi_i$ .

## 3.2 Two-Dimensional Spaces

A general vector state is written as a superposition of the basis states (3.5):

$$\begin{aligned} \Psi &= c_a \varphi_a + c_b \varphi_b \\ \varphi_a &= \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \varphi_b = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \end{aligned} \quad (3.15)$$

We define the Hermitian, traceless, Pauli matrices  $\sigma_i$  ( $i = x, y, z$ )

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \mathcal{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \quad (3.16)$$

They all square to the unit matrix  $\mathcal{I}$ . The basis states (3.15) are eigenstates of  $\sigma_z$  with eigenvalues  $\pm 1$ .

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<sup>2</sup>If several roots have the same eigenvalue, more equations should be discarded to get a non-homogeneous set of equations.

The most general observable can be written as a linear combination of the matrices (3.16) with real parameters  $\kappa_0, \kappa_i$

$$\hat{Q} = \kappa_0 \mathcal{I} + \sum_i \kappa_i \sigma_i. \quad (3.17)$$

The two-component states satisfy the eigenvalue equation

$$\begin{pmatrix} \langle a|Q|a\rangle & \langle a|Q|b\rangle \\ \langle b|Q|a\rangle & \langle b|Q|b\rangle \end{pmatrix} \begin{pmatrix} c_a \\ c_b \end{pmatrix} = q_{\pm} \begin{pmatrix} c_a \\ c_b \end{pmatrix}, \quad (3.18)$$

where  $\langle a|Q|a\rangle = \kappa_0 + \kappa_z$ ,  $\langle b|Q|b\rangle = \kappa_0 - \kappa_z$  and  $\langle a|Q|b\rangle = \langle b|Q|a\rangle^* = \kappa_x - i\kappa_y$ . The resulting eigenvalues are

$$q_{\pm} = \frac{1}{2} (\langle a|Q|a\rangle + \langle b|Q|b\rangle) \pm \frac{1}{2} \sqrt{(\langle a|Q|a\rangle - \langle b|Q|b\rangle)^2 + 4|\langle a|Q|b\rangle|^2}, \quad (3.19)$$

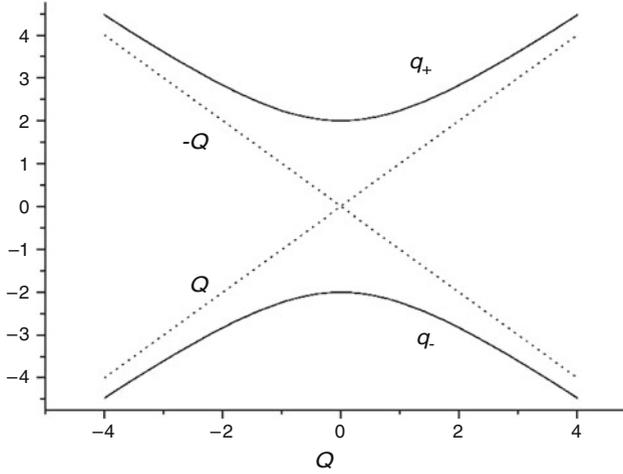
while the amplitudes of the eigenvectors are given by

$$\left. \frac{c_b}{c_a} \right|_{\pm} = \frac{q_{\pm} - \langle a|Q|a\rangle}{\langle a|Q|b\rangle}, \quad (c_a)_{\pm} = \left( 1 + \left| \frac{c_b}{c_a} \right|_{\pm}^2 \right)^{-\frac{1}{2}}. \quad (3.20)$$

Figure 3.1 plots the eigenvalues  $q_{\pm}$  and the initial expectation values as functions of  $Q \equiv \langle a|Q|a\rangle$ , assuming a traceless situation ( $\langle a|Q|a\rangle = -\langle b|Q|b\rangle$ ) and  $\langle a|Q|b\rangle = 2$ . The eigenvalue  $q_+$  is always higher than  $|Q|$ , while  $q_-$  is always below  $-|Q|$ : the two eigenvalues repel each other and never cross, if  $\langle a|Q|b\rangle \neq 0$ . The distance  $\Delta = \sqrt{Q^2 + |\langle a|Q|b\rangle|^2} - Q$  measures the increase in the highest eigenvalue of  $Q$ , due to the superposition of the states  $\phi_a, \phi_b$ , and it is maximized at the crossing point  $Q = 0$ .

The physical world displays many systems with two states, the spin being the most conspicuous one. But in fact, any two states sufficiently isolated from the remaining ones may be approximated as a two-state system, for which the no-crossing rule holds. Another example is given by an electron and two protons. As a reasonable approximation, we may neglect the motion of the protons, since they are much heavier than the electron. The two states  $\phi_a, \phi_b$  represent the electron bound to each of the protons: a hydrogen atom and a separate proton in each case. In this case the Hamiltonian  $\hat{H}$  plays the role of  $\hat{Q}$  in (3.18) and (3.19). The extra binding  $\Delta$ , arising from the superposition of states  $\phi_a, \phi_b$ , allows for the existence of a bound state: the stability of the ionized hydrogen molecule thus has a purely quantum mechanical origin. This problem is discussed in more detail in Sect. 8.4.1.

Let us consider the case  $\hat{Q} = \sigma_x$ . Equation (3.19) yields the eigenvalues  $s_x = \pm 1$  and the eigenvectors



**Fig. 3.1** Eigenvalues  $q_{\pm}$  of a  $2 \times 2$  system (continuous curves) as functions of  $Q$ , half of the energy distance between the diagonal matrix elements (dotted lines)

$$\begin{aligned}\phi_a^{(x)} &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}}\phi_a + \frac{1}{\sqrt{2}}\phi_b, \\ \phi_b^{(x)} &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \frac{1}{\sqrt{2}}\phi_a - \frac{1}{\sqrt{2}}\phi_b.\end{aligned}\quad (3.21)$$

These equations express the eigenstates of  $\sigma_x$  as linear combinations of the eigenstates (3.15) of  $\sigma_z$ . The relevance of the relative sign is apparent, in spite of the fact that the probability of obtaining any component of  $\sigma_z$  is the same for both cases.

The unitary transformation

$$\mathcal{U} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \quad (3.22)$$

transforms the basis set of eigenvectors of the operator  $\sigma_z$  into the basis set of eigenvectors of  $\sigma_x$ , in accordance with (3.14)

$$\mathcal{U} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad \mathcal{U} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}. \quad (3.23)$$

Similarly, the operator  $\sigma_z$  is transformed into the operator  $\sigma_x$  [see (2.14)]

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \mathcal{U} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \mathcal{U}^+. \quad (3.24)$$

It happens that the operators representing the spin components are given by  $\hat{S}_i = \frac{\hbar}{2}\sigma_i$ . Thus, the fact that the eigenvalues of  $\sigma_z$  are the same as those of  $\sigma_x$  is to be expected for physical reasons: the eigenvalues do indeed have physical significance, while the orientation of the coordinate system in an isotropic space does not.

### 3.3 Harmonic Oscillator

Here we present a solution to the harmonic oscillator problem, a solution that stems directly from the basic principles listed in Sect. 2.3. The Hamiltonian corresponding to the one-dimensional harmonic oscillator is

$$\hat{H} = \frac{1}{2M}\hat{p}^2 + \frac{M\omega^2}{2}\hat{x}^2, \quad (3.25)$$

where  $\omega$  is the classical frequency (Fig. 3.2).

The harmonic oscillator potential is probably the most widely used potential in physics, because of its ability to represent physical potentials in the vicinity of stable equilibrium [e.g. vibrational motion in molecules (8.28)].

It is always convenient to start by finding the order of magnitude of the quantities involved. To do so, we apply the Heisenberg uncertainty principle (2.37). If the substitutions  $\hat{x} \rightarrow \Delta x$  and  $\hat{p} \rightarrow \hbar/2\Delta x$  are made in the harmonic oscillator energy, so that

$$E \geq \frac{\hbar^2}{8M(\Delta x)^2} + \frac{M\omega^2(\Delta x)^2}{2}, \quad (3.26)$$

then minimization with respect to  $\Delta x$  gives the value at the minimum:

$$(\Delta x)_{\min} = \sqrt{\frac{\hbar}{2M\omega}}, \quad (3.27)$$

which yields the characteristic orders of magnitude

$$x_c = \sqrt{\frac{\hbar}{M\omega}}, \quad p_c = \sqrt{\hbar M\omega}, \quad E_c = \hbar\omega. \quad (3.28)$$

#### 3.3.1 Solution of the Eigenvalue Equation

We intend to solve (2.17). The unknowns are the eigenvalues  $E_i$  and the eigenfunctions  $\varphi_i$ . The fundamental tool entering the present solution is the commutation relation (2.15).

We first define the operators  $a^+$ ,  $a$

$$a^+ \equiv \sqrt{\frac{M\omega}{2\hbar}}\hat{x} - \frac{i}{\sqrt{2M\hbar\omega}}\hat{p}, \quad a \equiv \sqrt{\frac{M\omega}{2\hbar}}\hat{x} + \frac{i}{\sqrt{2M\hbar\omega}}\hat{p}. \quad (3.29)$$

The operators  $\hat{x}$  and  $\hat{p}$  are Hermitian, since they correspond to physical observables. Therefore, the operators  $a, a^+$  are Hermitian conjugates of each other, according to (2.50). They satisfy the commutation relations

$$[\hat{H}, a^+] = \hbar\omega a^+, \quad (3.30)$$

$$[a, a^+] = 1. \quad (3.31)$$

We now construct the matrix elements (2.10) for both sides of (3.30), making use of two eigenstates  $\varphi_i, \varphi_j$ :

$$\langle i | [\hat{H}, a^+] | j \rangle = (E_i - E_j) \langle i | a^+ | j \rangle = \hbar\omega \langle i | a^+ | j \rangle. \quad (3.32)$$

We conclude that the matrix element  $\langle i | a^+ | j \rangle$  vanishes, unless the difference  $E_i - E_j$  between the energies of the two eigenstates is the constant  $\hbar\omega$ . This fact implies that we may sequentially order the eigenstates connected by  $a^+$ , the difference between two consecutive energies being  $\hbar\omega$ . Another consequence is that we may assign an integer number  $n$  to each eigenstate.

Since  $a, a^+$  are Hermitian conjugate operators, we may also write

$$\langle n+1 | a^+ | n \rangle = \langle n | a | n+1 \rangle^*. \quad (3.33)$$

Finally, we expand the expectation value of (3.31):

$$\begin{aligned} 1 &= \langle n | [a, a^+] | n \rangle \\ &= \langle n | a | n+1 \rangle \langle n+1 | a^+ | n \rangle - \langle n | a^+ | n-1 \rangle \langle n-1 | a | n \rangle \\ &= |\langle n+1 | a^+ | n \rangle|^2 - |\langle n | a^+ | n-1 \rangle|^2. \end{aligned} \quad (3.34)$$

This is a finite difference equation in  $y_n = |\langle n+1 | a^+ | n \rangle|^2$ , of the type  $1 = y_n - y_{n-1}$ . Its solutions are

$$|\langle n+1 | a^+ | n \rangle|^2 = n + c, \quad \langle n+1 | a^+ | n \rangle = \sqrt{n+1}, \quad (3.35)$$

where  $c$  is a constant. Since the left-hand side is positive definite, the quantum number  $n$  must have a lower limit, which we may choose to be  $n = 0$ . It corresponds to the ground state  $\varphi_0$ . In such a case, the matrix element  $\langle 0 | a^+ | -1 \rangle$  should disappear, which fixes the value of the constant  $c = 1$ . Therefore, according to (3.33),  $\langle -1 | a | 0 \rangle = 0$ , which is equivalent to

$$a \varphi_0 = 0, \quad (3.36)$$

i.e. the ground state is annihilated by the operator  $a$ , which is called the annihilation operator.

The whole set of orthogonal eigenstates may be constructed by repeatedly applying the operator  $a^+$ , the creation operator:

$$\varphi_n = \frac{1}{\sqrt{n!}} (a^+)^n \varphi_0, \quad n = 0, 1, \dots \quad (3.37)$$

These states are labeled with the quantum number  $n$ . They are eigenstates of the operator  $\hat{n} = a^+ a$ , the number operator, with eigenvalues  $n$ :

$$\hat{n} \varphi_n = \frac{1}{\sqrt{n!}} a^+ [a, (a^+)^n] \varphi_0 = \frac{1}{\sqrt{n!}} a^+ n (a^+)^{n-1} \varphi_0 = n \varphi_n. \quad (3.38)$$

The factor  $1/\sqrt{n!}$  ensures the normalization of the eigenstates.

To find the matrix elements of the operators  $\hat{x}$  and  $\hat{p}$ , we invert the definition in (3.29):

$$\hat{x} = \sqrt{\frac{\hbar}{2M\omega}} (a^+ + a), \quad \hat{p} = i\sqrt{\frac{M\hbar\omega}{2}} (a^+ - a), \quad (3.39)$$

and obtain the non-vanishing matrix elements

$$\langle n+1|x|n\rangle = \langle n|x|n+1\rangle = \sqrt{\frac{\hbar}{M\omega} \frac{n+1}{2}}, \quad (3.40)$$

$$\langle n+1|p|n\rangle = \langle n|p|n+1\rangle^* = i\sqrt{M\hbar\omega} \frac{n+1}{2}. \quad (3.41)$$

Substitution of (3.39) into the Hamiltonian yields

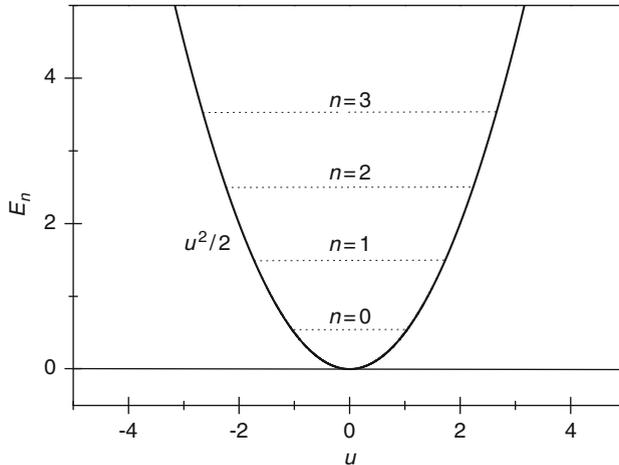
$$\hat{H} = \hbar\omega \left( \hat{n} + \frac{1}{2} \right), \quad (3.42)$$

where the operator  $\hat{n}$  has the quantum number  $n$  ( $= 0, 1, 2, \dots$ ) as eigenvalues. Thus, the Hamiltonian matrix is diagonal, with eigenvalues  $E_n$  represented in Fig. 3.2

$$\langle n|H|n\rangle = E_n = \hbar\omega \left( n + \frac{1}{2} \right). \quad (3.43)$$

The creation and annihilation operators are often used in many-body quantum physics (Sects. 7.4.4<sup>†</sup> and 7.8<sup>†</sup>). They are also essential tools in quantum field theory, since they allow us to represent the creation and annihilation of phonons, photons, mesons, etc. (Sects. 9.8.2<sup>†</sup> and 9.8.3<sup>†</sup>).

Quantum mechanics has provided the present derivation based on the fundamental commutation relation (2.15), which yield the properties of the matrix elements



**Fig. 3.2** Harmonic oscillator potential and its eigenvalues. All energies are given in units of  $\hbar\omega$ . The dimensionless variable  $u = x/x_c$  has been used

$|n\rangle a^+ |m\rangle$  in a straightforward way. The results are also valid for any problem involving two operators satisfying (2.15), with a Hamiltonian that is quadratic in these operators.

### 3.3.2 Some Properties of the Solution

In the following we use this exact, analytical solution of the harmonic oscillator problem to deduce some relevant features of quantum mechanics.<sup>3</sup> The discussion of the spatial dependence of the harmonic oscillator problem is deferred to Sect. 4.2.

- The classical equilibrium position  $x = p = 0$  is not compatible with the uncertainty principle, because it implies a simultaneous determination of coordinate and momentum. The replacement of  $\Delta x$  in (3.26) with (3.27) yields the zero-point energy<sup>4</sup> (3.43)

$$E_0 = \frac{1}{2}\hbar\omega, \quad (3.44)$$

<sup>3</sup>However, the reader is warned against concluding that most quantum problems are analytically solvable, a conclusion that may be reinforced throughout these notes by the repeated utilization of exactly soluble examples. Most quantum problems require insight into physics to approximate the solution and/or sizeable computing facilities.

<sup>4</sup>The procedure is only expected to yield correct orders of magnitude. It is a peculiarity of the harmonic oscillator that the results are exact.

i.e. the minimum energy that the harmonic oscillator may have. This purely quantum effect was observed even before the invention of quantum mechanics. Roger Mulliken showed in 1924 that the inclusion of (3.44) leads to a better agreement with data obtained by comparing the vibrational spectra (see Sect. 8.4.2) of two molecules made up from different isotopes of the same element [29]. Applications of the zero-point energy concept range from the explanation of the intermolecular Van der Waals force (Problem 11, Chap. 8) to speculations about massive effects of the electromagnetic vacuum represented by the ground state of infinite harmonic oscillators (Sect. 9.8.2<sup>†</sup>).

- By using the closure property (2.59) and the matrix elements (3.40) and (3.41), one obtains the matrix element of the commutator  $[\hat{x}, \hat{p}]$ :

$$\begin{aligned} \langle n|[x, p]|m\rangle &= \langle n|x|n+1\rangle\langle n+1|p|m\rangle + \langle n|x|n-1\rangle\langle n-1|p|m\rangle \\ &\quad - \langle n|p|n+1\rangle\langle n+1|x|m\rangle - \langle n|p|n-1\rangle\langle n-1|x|m\rangle \\ &= i\hbar\delta_{nm}. \end{aligned} \quad (3.45)$$

The matrix elements of the operators  $\hat{x}^2$  and  $\hat{p}^2$  may be constructed in a similar way:

$$\frac{M\omega}{\hbar}\langle n|x^2|n\rangle = \frac{1}{\hbar M\omega}\langle n|p^2|n\rangle = n + \frac{1}{2}, \quad (3.46)$$

which implies the equality between the kinetic energy and potential expectation values (virial theorem).

Applying the definition of the root mean square deviation  $\Delta Q$  given in (2.20), the product  $\Delta x\Delta p$  yields

$$(\Delta x)_n(\Delta p)_n = \frac{E_n}{\omega} = \hbar\left(n + \frac{1}{2}\right) \geq \frac{1}{2}\hbar. \quad (3.47)$$

This inequality expresses the uncertainty principle (Sect. 2.6.1). We have thus verified the intimate connection between the commutation relation of two operators and the uncertainties in the measurement of the corresponding physical quantities.

- The invariance with respect to the parity transformation  $\hat{\Pi}$  ( $x \rightarrow -x$ ) plays an important role in quantum mechanics. The fact that neither the kinetic energy nor the harmonic oscillator potential energy is altered by the parity transformation is expressed by the commutation relation

$$[\hat{H}, \hat{\Pi}] = 0. \quad (3.48)$$

As a consequence of this relation, it is possible to know simultaneously the eigenvalues of the two operators  $\hat{H}$ ,  $\hat{\Pi}$  (see Sect. 2.6.1). In this case the eigenstates of the harmonic oscillator Hamiltonian are also eigenstates of the parity operator  $\hat{\Pi}$ . The eigenvalues of the operator  $\hat{\Pi}$  are determined by the fact that the operator  $\hat{\Pi}^2$

must have the single eigenvalue  $\pi^2 = 1$ , since the system is left unchanged after two applications of the parity transformation. There are thus two eigenvalues corresponding to the operator  $\hat{\Pi}$ , namely  $\pi = \pm 1$ . The eigenfunctions are either invariant under the parity transformation ( $\pi = 1$ , even functions) or change sign ( $\pi = -1$ , odd functions). This is verified in the case of the harmonic oscillator, since the operators  $a^+$ ,  $a$  change sign under the parity transformation and the parity of the state labeled by the quantum number  $n$  is therefore

$$\hat{\Pi}\varphi_n = (-1)^n\varphi_n. \quad (3.49)$$

Symmetries constitute essential tools in the characterization and solution of quantum problems. Every symmetry gives rise to a new quantum number.

### 3.4 The Jaynes–Cummings Model

Consider a system consisting of a two-state atom coupled to a harmonic oscillator. The Hamiltonian of the uncoupled subsystems is

$$\hat{H}_0 = \frac{\hbar}{2} [\omega_a\sigma_z + \omega_{\text{ho}}(2\hat{n} + 1)]. \quad (3.50)$$

The eigenvalues of this Hamiltonian are organized as ladder doublets separated by the oscillator distance  $\hbar\omega_{\text{ho}}$ . The atom excitation energy is  $\hbar\omega_a$ . The eigenvectors of  $\hat{H}_0$  are given by the product states  $\varphi_a \chi_n$  and  $\varphi_b \chi_n$  [see (3.15) and (3.37)].

Let us introduce a coupling Hamiltonian

$$H_{\text{coup}} = -i\frac{\hbar}{2}\Omega (a\sigma_+ - a^+\sigma_-), \quad \sigma_{\pm} = \frac{1}{2}(\sigma_x \pm i\sigma_y), \quad (3.51)$$

which feeds the population of the upper atomic state with a simultaneous de-excitation of the oscillator, and vice versa. Therefore, it only displays a non-vanishing matrix element between the states  $\varphi_a \chi_n$  and  $\varphi_b \chi_{n+1}$ , which remain uncoupled from all other pairs. Aside from a common constant energy, the Hamiltonian of the pair is

$$\hat{H}_0 + \hat{H}_{\text{ho}} = \frac{\hbar}{2} (W\sigma_z + \Omega_n\sigma_y) = \frac{\hbar}{2} \begin{pmatrix} W & -i\Omega_n \\ i\Omega_n & -W \end{pmatrix}, \quad (3.52)$$

where  $W = \omega_a - \omega_{\text{ho}}$  and  $\Omega_n = \Omega \sqrt{n+1}$ . Since this is a particular case of the Hamiltonian (3.18), the discussion following that equation applies. In particular, the resulting eigenstates are of the form

$$\Psi_{\pm} = c_{an}^{(\pm)} \varphi_a \chi_n + c_{b(n+1)}^{(\pm)} \varphi_b \chi_{n+1}. \quad (3.53)$$

This simple Jaynes–Cummings model [30] is applicable to recent tests of quantum mechanics based on the interaction between a single atom and the electromagnetic field (Sect. 12.3.3).

## Problems

**Problem 1.** Consider the matrix

$$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}.$$

1. Find the eigenvalues and verify the conservation of the trace after diagonalization.
2. Find the eigenvector corresponding to each eigenvalue.
3. Check the orthogonality of states corresponding to different eigenvalues.
4. Construct the unitary transformation from the basic set of states used in (3.5) to the eigenstates of this matrix.

**Problem 2.** Consider the matrix

$$\begin{pmatrix} a & c \\ c & -a \end{pmatrix}.$$

1. Calculate the eigenvalues as functions of the real numbers  $a, c$ .
2. Show that the odd terms in  $c$  vanish in an expansion in powers of  $c$  ( $|c| \ll |a|$ ).
3. Show that the linear term does not disappear if  $|c| \gg |a|$ .

**Problem 3.** Which of the following vector states are linearly independent?

$$\varphi_1 = \begin{pmatrix} i \\ 1 \end{pmatrix}, \quad \varphi_2 = \begin{pmatrix} -i \\ 1 \end{pmatrix}, \quad \varphi_3 = \begin{pmatrix} 1 \\ i \end{pmatrix}, \quad \varphi_4 = \begin{pmatrix} 1 \\ -i \end{pmatrix}.$$

**Problem 4.** Consider the two operators

$$\hat{Q} = \begin{pmatrix} 0.5 & 0 & 0 \\ 0 & 0.5 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad \text{and} \quad \hat{R} = \begin{pmatrix} 0 & 0.5 & 0 \\ 0.5 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

1. Calculate the eigenvalues.
2. Determine whether or not the operators commute.
3. If so, obtain the simultaneous eigenvectors of both operators.

**Problem 5.** Consider a unit vector with components  $\cos \beta$  and  $\sin \beta$  along the  $z$ - and  $x$ -axes, respectively. The matrix representing the spin operator in this direction is written as  $\hat{S}_\beta = \hat{S}_z \cos \beta + \hat{S}_x \sin \beta$ .

1. Find the eigenvalues of  $\hat{S}_\beta$  using symmetry properties.
2. Diagonalize the matrix.
3. Find the amplitudes of the new eigenstates in a basis for which the operator  $\hat{S}_z$  is diagonal.

**Problem 6.** If  $a$  and  $a^+$  are the annihilation and creation operators defined in (3.29), show that  $[a, (a^+)^n] = n(a^+)^{n-1}$ .

**Problem 7.** 1. Calculate the energy of a particle subject to the potential  $V(x) = V_0 + c\hat{x}^2/2$  if the particle is in the third excited state.  
2. Calculate the energy eigenvalues for a particle moving in the potential  $V(x) = c\hat{x}^2/2 + b\hat{x}$ .

**Problem 8.** 1. Express the distance  $x_c$  as a function of the mass  $M$  and the restoring parameter  $c$  used in Problem 7.  
2. If  $c$  is multiplied by 9, what is the separation between consecutive eigenvalues?  
3. Show that  $x_c$  is the maximum displacement of a classical particle moving in a harmonic oscillator potential with an energy of  $\hbar\omega/2$ .

**Problem 9.** Evaluate the matrix elements  $\langle n + \eta | x^2 | n \rangle$  and  $\langle n + \eta | p^2 | n \rangle$  in the harmonic oscillator basis for  $\eta = 1, 2, 3, 4$ :

1. Using the closure property and the matrix elements (3.41)
2. Applying the operators  $\hat{x}^2$  and  $\hat{p}^2$ , expressed in terms of the  $a^+, a$ , on the eigenstates (3.37)

Find the ratio  $\langle n + \nu | K | n \rangle : \langle n + \nu | V | n \rangle$  ( $\nu = 0, \pm 2$ ) in the harmonic oscillator basis, where  $\hat{K}, \hat{V}$  are the operators corresponding to the kinetic and the potential energies, respectively. Justify the resulting sign difference between these three cases on quantum mechanical grounds.

**Problem 10.** Calculate the expectation value of the coordinate operator for a linear combination of harmonic oscillator states with the same parity.

**Problem 11.** 1. Construct the normalized, linear combination of harmonic oscillator states  $\Psi = c_0\phi_0 + c_1\phi_1$  for which the expectation value  $\langle \Psi | x | \Psi \rangle$  becomes maximized.  
2. Evaluate in such a state the expectation values of the coordinate, the momentum and the parity operators.

Note: In some chemical bonds, nature takes advantage of the fact that electrons protrude from the atom in a state similar to the linear combination  $\Psi$ . This situation is called hybridization.

**Problem 12.** Verify the normalization of the states (3.37).

**Problem 13.** Find the amplitudes  $c_i^{(\pm)}$  in (3.53) for the resonant case  $\omega_a = \omega_{\text{ho}}$ .