Appendix A

Quantum mechanics and phase-space

A.1 Fundamentals of quantum mechanics

A.1.1 Pure states and operators

The state of a quantum-mechanical system corresponding to maximal knowledge is known as a *pure* state. It is represented by a vector in Hilbert space $\mathbb{H}$, a complex vector space with an arbitrarily large dimensionality. We use Dirac's notation and write the basis vectors for the Hilbert space as $|\phi_j\rangle$ for $j \in \{0, 1, 2, \ldots, D-1\}$. Strictly the formulation we present below holds only for finite D, but the generalizations for infinite D present few problems, although there are some traps for the unwary. For a fuller discussion, see, for example, the excellent book by Ballentine [Bal98].

We define an inner product on the Hilbert space so that the basis states are orthonormal: $\langle\phi_i|\phi_j\rangle = \delta_{ij}$. Then, for a complete basis, we can write an arbitrary pure state, or *state vector*, or *ket* as

$$|\psi\rangle = \sum_i \psi_i |\phi_i\rangle, \tag{A.1}$$

where, for all i, $\psi_i \in \mathbb{C}$ (the complex numbers). The dual vector, or *bra*, is defined as

$$\langle\psi| = \sum_i \psi_i^* \langle\phi_i|. \tag{A.2}$$

If the state vector is to be normalized we require the inner product, or *bracket*, to satisfy

$$\langle\psi|\psi\rangle = \sum_i |\psi_i|^2 = 1. \tag{A.3}$$

In order to relate the state to quantities of physical interest, we need to introduce *operators*. An operator is an object that maps a Hilbert space onto itself, and so can be written in Dirac notation as

$$\hat{A} = \sum_{ij} A_{ij} |\phi_i\rangle\langle\phi_j|, \tag{A.4}$$

where the A_{ij} are complex numbers. Operators are sometimes called q-numbers, meaning quantum numbers, as opposed to c-numbers, which are ordinary classical or complex numbers. Ignoring some subtle issues to do with infinite-dimensional Hilbert spaces, we can simply state that all physical quantities (commonly called *observables*) are associated with *Hermitian* operators. An Hermitian operator is one that is equal to its Hermitian

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adjoint, defined as

$$\hat{A}^\dagger = \sum_{ij} A^*_{ji} |\phi_i\rangle\langle\phi_j|. \tag{A.5}$$

In matrix terms, $A = (A^*)^\top$. In Table A.1 we summarize definitions such as these and their relations to linear algebra. A knowledge of the results in this table is assumed in subsequent discussions.

If $\hat{\Lambda}$ is the operator which represents a physical quantity Λ, then the simplest connection we can make with the state of the system $|\psi\rangle$ is that the mean value of Λ is given by

$$\langle\Lambda\rangle = \langle\psi|\hat{\Lambda}|\psi\rangle, \tag{A.6}$$

where, unless otherwise stated, we take the ket to be normalized. We derive this expression from more basic considerations in Section 1.2.2.

Note that Eq. (A.6) shows that the *absolute* phase of a state plays no physical role; $e^{i\phi}|\psi\rangle$ gives the same mean value for all observables as does $|\psi\rangle$. Of course the *relative* phase of states in a superposition *does* matter. That is, for a state such as $e^{i\phi_1}|\psi_1\rangle + e^{i\phi_2}|\psi_2\rangle$, the average value of physical quantities will depend in general upon $\phi_2 - \phi_1$.

Exercise A.1 *Convince yourself of these statements.*

Any Hermitian operator $\hat{\Lambda}$ can be diagonalized as

$$\hat{\Lambda} = \sum_\lambda \lambda|\lambda\rangle\langle\lambda|, \tag{A.7}$$

where $\{\lambda\}$ are the eigenvalues of $\hat{\Lambda}$ which are real, while $\{|\lambda\rangle\}$ forms a complete basis. Here for simplicity we have taken the spectrum – the set of eigenvalues – to be discrete and non-degenerate (that is, all eigenvalues are different).

Exercise A.2 *Using this representation, show that* $\langle\Lambda\rangle$ *is real.*

If we assume that the operator for Λ^2 is $\hat{\Lambda}^2$ (which is justified in Section 1.2.2), then it is not difficult to show that the variance in Λ,

$$\mathrm{Var}[\Lambda] = \langle\psi|\hat{\Lambda}^2|\psi\rangle - \langle\psi|\hat{\Lambda}|\psi\rangle^2, \tag{A.8}$$

is in general greater than zero. This is the puzzling phenomenon of quantum noise; even though we have a state of maximal knowledge about the system, there is still some uncertainty in the values of physical quantities. Moreover, it is possible to derive so-called *uncertainty relations* of the form

$$\mathrm{Var}[\Lambda]\mathrm{Var}[\mathrm{B}] \geq |\langle\psi|[\hat{\Lambda}, \hat{\mathrm{B}}]|\psi\rangle|^2/4, \tag{A.9}$$

where $[\hat{\Lambda}, \hat{\mathrm{B}}] \equiv \hat{\Lambda}\hat{\mathrm{B}} - \hat{\mathrm{B}}\hat{\Lambda}$ is called the commutator. If the commutator is a c-number (that is, it is proportional to the identity operator), this relation puts an absolute lower bound on the product of the two uncertainties.

Exercise A.3 *The position Q and momentum P of a particle have operators that obey $[\hat{P}, \hat{Q}] = -i\hbar$ (see Section A.3). Using Eq. (A.9), derive Heisenberg's uncertainty relation*

$$\left\langle(\Delta P)^2\right\rangle\left\langle(\Delta Q)^2\right\rangle \geq (\hbar/2)^2, \tag{A.10}$$

where $\Delta P = P - \langle P\rangle$ and similarly for Q.

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Table A.1. *Linear algebra and quantum mechanics*

Linear algebra		Quantum operator algebra	
$\mathbb{H}$	Complex vector space	$\mathbb{H}$	Hilbert space
$\dim(\mathbb{H})$	dimension D	$\dim(\mathbb{H})$	dimension D
A	Matrix	$\hat{A}$	Operator
$\vec{v}$	Column vector	$\|\psi\rangle$	State vector or ket
$(\vec{v}^{\,*})^\top$	Conjugate row vector	$\langle\psi\|$	Bra
$(\vec{v}^{\,*})^\top\vec{u}$	Inner or dot product $\vec{v}\cdot\vec{u}$	$\langle\psi\|\theta\rangle$	Inner product
$\vec{v}\cdot\vec{u}=0$	Orthogonality	$\langle\psi\|\theta\rangle=0$	Orthogonality
$\vec{v}\cdot\vec{v}=1$	Unit vector	$\langle\psi\|\psi\rangle=1$	Normalized state vector
$\vec{u}(\vec{v}^{\,*})^\top$	Outer product (a matrix)	$\|\theta\rangle\langle\psi\|$	Outer product (an operator)
$\{\vec{\alpha}\}$	Eigenvectors $A\vec{\alpha}=\alpha\vec{\alpha}$	$\{\|\alpha\rangle\}$	Eigenstates $\hat{A}\|\alpha\rangle=\alpha\|\alpha\rangle$
$\{\alpha\}$	Eigenvalues (complex)	$\{\alpha\}$	Eigenvalues (complex)
$(A^*)^\top$	Hermitian adjoint	$\hat{A}^\dagger$	Hermitian adjoint
U	Unitary matrix $(U^*)^\top=U^{-1}$	$\hat{U}$	Unitary operator $\hat{U}^\dagger=\hat{U}^{-1}$
Λ	Hermitian matrix $\Lambda=(\Lambda^*)^\top$ $\Longrightarrow\{\lambda\}$ Real eigenvalues $\Longrightarrow\{\vec{\lambda}\}$ Orthogonal eigenvectors	$\hat{\Lambda}$	Hermitian operator $\hat{\Lambda}=\hat{\Lambda}^\dagger$ $\Longrightarrow\{\lambda\}$ Real eigenvalues $\Longrightarrow\{\|\lambda\rangle\}$ Orthogonal eigenstates
$\{\vec{e}_j\}_{j=0}^{D-1}$	Orthonormal basis $\Longrightarrow\vec{e}_j\cdot\vec{e}_k=\delta_{jk}$	$\{\|\phi_j\rangle\}_{j=0}^{D-1}$	Orthonormal basis $\Longrightarrow\langle\phi_j\|\phi_k\rangle=\delta_{jk}$
U	Change of basis $\vec{e}_j{}'=\sum_k U_{jk}\vec{e}_k$	$\hat{U}$	Change of basis $\|\phi_j'\rangle=\sum_k U_{jk}\|\phi_k\rangle$
I	Identity $\sum_j(\vec{e}^{\,*}_j)\vec{e}_j^{\,\top}$	$\hat{1}$	Identity $\sum_j\|\phi_j\rangle\langle\phi_j\|$
v_j	Vector component $\vec{e}_j\cdot\vec{v}$	ψ_j	Probability amplitude $\psi_j=\langle\phi_j\|\psi\rangle$
A_{jk}	Matrix element $(\vec{e}_j{}^{\,*})^\top A\vec{e}_k$	A_{jk}	Matrix element $\langle\phi_j\|\hat{A}\|\phi_k\rangle$
$\mathrm{tr}\,A$	Trace $\sum_j A_{jj}$	$\mathrm{Tr}[\hat{A}]$	Trace $\sum_j\langle\phi_j\|\hat{A}\|\phi_j\rangle$
$\mathbb{H}=\mathbb{H}_1\otimes\mathbb{H}_2$	Tensor product $\Longrightarrow D=\dim(\mathbb{H})=D_1\times D_2$	$\mathbb{H}=\mathbb{H}_1\otimes\mathbb{H}_2$	Tensor product $\Longrightarrow D=\dim(\mathbb{H})=D_1\times D_2$
$\vec{v}_1\otimes\vec{u}_2$	Tensor product $\Longrightarrow\vec{E}_{k\times D_2+j}=(\vec{e}_k)_1\otimes(\vec{e}_j)_2$	$\|\psi\rangle_1\otimes\|\theta\rangle_2$	Tensor product $\|\psi\rangle_1\|\theta\rangle_2$ $\Longrightarrow\|\Phi_{k\times D_2+j}\rangle=\|\phi_k\rangle_1\otimes\|\phi_j\rangle_2$
$A_1\otimes B_2$	Tensor product $\Longrightarrow A_1\otimes B_2[\vec{v}_1\otimes\vec{u}_2]=$ $(A_1\vec{v}_1)\otimes(B_2\vec{u}_2)$	$\hat{A}_1\otimes\hat{B}_2$	Tensor product $\Longrightarrow\hat{A}_1\otimes\hat{B}_2[\|\psi\rangle_1\otimes\|\theta\rangle_2]=$ $\hat{A}_1\|\psi\rangle_1\otimes\hat{B}_2\|\theta\rangle_2$

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A.1.2 Mixed states

The pure states considered so far are appropriate only if one knows everything one can know about the system. It is easy to imagine situations in which this is not the case. Suppose one has a physical device that prepares a system in one of N states, $|\psi_j\rangle$: $j = 1, \ldots, N$, with corresponding probabilities $\wp_j$. These states need not be orthogonal, and N can be greater than the dimension of the Hilbert space of the system. We will call the action of this device a *preparation procedure* and the set $\{\wp_j, |\psi_j\rangle: j = 1, 2, \ldots, N\}$ an *ensemble* of pure states.

If one has no knowledge of which particular state is produced, the expected value of a physical quantity is clearly the weighted average

$$\langle \Lambda \rangle = \sum_j \wp_j \langle \psi_j | \hat{\Lambda} | \psi_j \rangle. \tag{A.11}$$

We can combine the classical and quantum expectations in a single entity by defining a new operator. This is called (for historical reasons) the density operator, and is given by

$$\rho = \sum_{j=1}^{N} \wp_j |\psi_j\rangle\langle\psi_j|. \tag{A.12}$$

We can then write

$$\langle \Lambda \rangle = \mathrm{Tr}\big[\rho \hat{\Lambda}\big], \tag{A.13}$$

where the trace operation is defined in Table A.1.

Exercise A.4 *Show this, by first showing that* $\mathrm{Tr}[|\psi\rangle\langle\theta|] = \langle\theta|\psi\rangle$.

The density operator is also known as the *density matrix*, or (in analogy with the state vector) the *state matrix*. It is the most general representation of a quantum state and encodes all of the physical meaningful information about the preparation of the system. Because of its special role, the state matrix is the one operator which we do not put a hat on.

The state matrix ρ is positive: all of its eigenvalues are non-negative. Strictly, it is a positive semi-definite operator, rather than a positive operator, because some of its eigenvalues may be zero. The eigenvalues also sum to unity, since

$$\mathrm{Tr}[\rho] = \sum_j \wp_j = 1. \tag{A.14}$$

In the case in which the ensemble of state vectors has only one element, ρ represents a pure state. In that case it is easy to verify that $\rho^2 = \rho$. Moreover, this condition is sufficient for ρ to be a pure state, since $\rho^2 = \rho$ means that ρ is a projection operator (these are discussed in Section 1.2.2). Using the normalization condition (A.14), it follows that ρ must be a rank-1 projection operator, which we denote as $\hat{\pi}$. That is to say, it must be of the form

$$\rho = |\psi\rangle\langle\psi| \tag{A.15}$$

for some ket $|\psi\rangle$. A state that cannot be written in this form is often called a *mixed* or *impure* state. The 'mixedness' of ρ can be measured in a number of ways. For instance, the *impurity* is usually defined to be one minus the *purity*, where the latter is $p = \mathrm{Tr}\big[\rho^2\big]$.

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Exercise A.5 *Show that* $0 \leq p \leq 1$, *with* $p = 1$, *if and only if* ρ *is pure.*
Hint: *The trace of the matrix* ρ^2 *is most easily evaluated in the diagonal basis for* ρ.

Alternatively, one can define the von Neumann entropy

$$S(\rho) = -\mathrm{Tr}[\rho \log \rho] \geq 0, \tag{A.16}$$

where the equality holds if and only if ρ is pure. To obtain a quantity with the dimensions of thermodynamic entropy, it is necessary to multiply it by Boltzmann's constant k_{B}.

An interesting point about the definition (A.12) is that it is not possible to go backwards from ρ to the ensemble of state vectors $\{\wp_j, |\psi_j\rangle : j = 1, 2, \ldots, N\}$. Indeed, for any Hilbert space, there is an uncountable infinity of ways in which any impure state matrix ρ can be decomposed into a convex (i.e. positively weighted) ensemble of rank-1 projectors. This is quite different from classical mechanics, in which different ensembles of states of complete knowledge correspond to different states of incomplete knowledge. Physically, we can say that any mixed quantum state admits infinitely many preparation procedures.

The non-unique decomposition of a state matrix can be shown up quite starkly using a two-dimensional Hilbert space: an electron drawn randomly from an ensemble in which half are spin up and half are spin down is *identical* to one drawn from an ensemble in which half are spin left and half spin right. No possible experiment can distinguish between them.

Exercise A.6 *Show this by showing that the state matrix under both of these preparation procedures is proportional to the identity.*
Hint: *If the up and down spin basis states are* $|\uparrow\rangle$ *and* $|\downarrow\rangle$, *the left and right spin states are* $|\rightarrow\rangle = (|\uparrow\rangle + |\downarrow\rangle)/\sqrt{2}$ *and* $|\leftarrow\rangle = (|\uparrow\rangle - |\downarrow\rangle)/\sqrt{2}$.

In this case, it is because the state matrix has degenerate eigenvalues that it is possible for both of these ensembles to comprise orthogonal states. If ρ has no degenerate eigenvalues, it is necessary to consider non-orthogonal ensembles to obtain multiple decompositions.

A.1.3 Time evolution

An isolated quantum system undergoes reversible evolution generated by an Hermitian operator called the Hamiltonian or energy operator $\hat{H}$. There are two basic ways of describing this time evolution, called the Schrödinger picture (SP) and the Heisenberg picture (HP). In the former, the state of the system changes but the operators are constant, whereas in the latter the state is time-independent and the operators are time-dependent.

Using units where $\hbar = 1$ (a convention we use in most places in this book, except for parts of Chapter 6), the SP evolution of the state matrix is

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = -\mathrm{i}[\hat{H}, \rho(t)]. \tag{A.17}$$

For pure states the corresponding equation (the Schrödinger equation) is

$$\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = -\mathrm{i}\hat{H}|\psi(t)\rangle. \tag{A.18}$$

It is easy to see that the solutions of these equations are

$$\rho(t) = \hat{U}(t, 0)\rho(0)\hat{U}^{\dagger}(t, 0), \qquad |\psi(t)\rangle = \hat{U}(t, 0)|\psi(0)\rangle, \tag{A.19}$$

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where $\hat{U}(t,0) = \exp(-\mathrm{i}\hat{H}t)$. This is called the unitary evolution operator, because it satisifes the unitarity conditions

$$\hat{U}^\dagger \hat{U} = \hat{U}\hat{U}^\dagger = \hat{1}. \tag{A.20}$$

If the Hamiltonian is a time-dependent operator $\hat{H}(t)$, as would arise from a classical external modulation of the system, then the evolution is still unitary. The evolution operator is

$$\hat{U}(t,0) = \hat{1} + \sum_{n=1}^{\infty} (-\mathrm{i})^n \int_0^t \mathrm{d}s_n\, \hat{H}(s_n) \int_0^{s_n} \mathrm{d}s_{n-1}\, \hat{H}(s_{n-1}) \cdots \int_0^{s_2} \mathrm{d}s_1\, \hat{H}(s_1). \tag{A.21}$$

Exercise A.7 *Show this, and show also that* $\hat{U}(t,0)$ *is unitary.*
Hint: *Assuming the solutions (A.19), derive the differential equation and initial conditions for* $\hat{U}(t,0)$ *and* $\hat{U}^\dagger(t,0)$*. Then show that Eq. (A.21) satisfies these, and that the unitarity conditions (A.20) are satisfied at* $t = 0$ *and are constants of motion.*

In the HP, the equation of motion for an arbitrary operator $\hat{A}$ is

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{A}(t) = +\mathrm{i}[\hat{H}(t), \hat{A}(t)]. \tag{A.22}$$

Note that, because $\hat{H}(t)$ commutes with itself at a particular time t, the Hamiltonian operator is one operator that is the same in both the HP and the SP. The solution of the HP equation is

$$\hat{A}(t) = \hat{U}^\dagger(t,0)\hat{A}(0)\hat{U}(t,0). \tag{A.23}$$

The two pictures are equivalent because all expectation values are identical:

$$\begin{aligned} \mathrm{Tr}\big[\hat{A}(t)\rho(0)\big] &= \mathrm{Tr}\big[\hat{U}^\dagger(t,0)\hat{A}(0)\hat{U}(t,0)\rho(0)\big] \\ &= \mathrm{Tr}\big[\hat{A}(0)\hat{U}(t,0)\rho(0)\hat{U}^\dagger(t,0)\big] \\ &= \mathrm{Tr}\big[\hat{A}(0)\rho(t)\big]. \end{aligned} \tag{A.24}$$

Here the placement of the time argument t indicates which picture we are in.

Often it is useful to split a Hamiltonian $\hat{H}$ into $\hat{H}_0 + \hat{V}(t)$, where $\hat{H}_0$ is time-independent and easy to deal with, while $\hat{V}(t)$ (which may be time-dependent) is typically more complicated. Then the unitary operator (A.21) can be written as

$$\hat{U}(t,0) = \mathrm{e}^{-\mathrm{i}\hat{H}_0 t}\hat{U}_{\mathrm{IF}}(t,0), \tag{A.25}$$

where $\hat{U}_{\mathrm{IF}}(t,0)$ is given by

$$\hat{1} + \sum_{n=1}^{\infty} (-\mathrm{i})^n \int_0^t \mathrm{d}s_n\, \hat{V}_{\mathrm{IF}}(s_n) \int_0^{s_n} \mathrm{d}s_{n-1}\, \hat{V}_{\mathrm{IF}}(s_{n-1}) \cdots \int_0^{s_2} \mathrm{d}s_1\, \hat{V}_{\mathrm{IF}}(s_1). \tag{A.26}$$

Here $\hat{V}_{\mathrm{IF}}(t) = \mathrm{e}^{\mathrm{i}\hat{H}_0 t}\hat{V}(t)\mathrm{e}^{-\mathrm{i}\hat{H}_0 t}$ and IF stands for 'interaction frame'.

Exercise A.8 *Show this, by showing that* $\mathrm{e}^{-\mathrm{i}\hat{H}_0 t}\hat{U}_{\mathrm{IF}}(t,0)$ *obeys the same differential equation as* $\hat{U}(t,0)$.

That is, one can treat $\hat{V}_{\mathrm{IF}}(t)$ as a time-dependent Hamiltonian, and then add the evolution $\mathrm{e}^{-\mathrm{i}\hat{H}_0 t}$ at the end. This can be used to define an *interaction picture* (IP), so called because

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$\hat{V}(t)$ is often the 'interaction Hamiltonian' coupling two systems, while $\hat{H}_0$ is the 'free Hamiltonian' of the uncoupled systems. The IP is a sort of half-way house between the SP and HP, usually defined so that operators evolve according to the unitary $\mathrm{e}^{-\mathrm{i}\hat{H}_0 t}$, while states evolve according to the unitary $\hat{U}_{\mathrm{IF}}(t,0)$. That is, one breaks up the expectation value for an observable A at time t as follows:

$$\langle A(t)\rangle = \mathrm{Tr}\big[\hat{U}^{\dagger}(t,0)\hat{A}(0)\hat{U}(t,0)\rho(0)\big] \tag{A.27}$$

$$= \mathrm{Tr}\Big[\Big\{\mathrm{e}^{\mathrm{i}\hat{H}_0 t}\,\hat{A}(0)\mathrm{e}^{-\mathrm{i}\hat{H}_0 t}\Big\}\Big\{\hat{U}_{\mathrm{IF}}(t,0)\rho(0)\hat{U}_{\mathrm{IF}}^{\dagger}(t,0)\Big\}\Big]. \tag{A.28}$$

An alternative approach to using the identity $\hat{U}(t,0) = \mathrm{e}^{-\mathrm{i}\hat{H}_0 t}\hat{U}_{\mathrm{IF}}(t,0)$ is simply to *ignore* the final $\exp(-\mathrm{i}\hat{H}_0 t)$ altogether, and just use $\hat{U}_{\mathrm{IF}}(t,0)$ as one's unitary evolution operator. The latter is often simpler, since $\hat{V}_{\mathrm{IF}}$ may often be made time-independent (even if $\hat{H}$ is explicitly time-dependent) by a judicious division into $\hat{H}_0$ and $\hat{V}$. If it cannot, then a *secular* or *rotating-wave* approximation is often used to make it time-independent (see Exercise 1.30).

We refer to the method of just using $\hat{U}_{\mathrm{IF}}$ as 'working in the interaction frame'. This terminology is used in analogy with, for example, 'working in a rotating frame' to calculate projectile trajectories on a rotating Earth. Working in the interaction frame is very common in quantum optics, where it is often (but incorrectly) called 'working in the interaction picture'. The interaction frame is not a 'picture' in the same way as the Heisenberg or Schrödinger picture. The HP or SP (or IP) includes the complete Hamiltonian evolution, whereas working in the interaction frame ignores the 'boring' free evolution. The interaction frame may contain either a Heisenberg or a Schrödinger picture, depending on whether $\hat{U}_{\mathrm{IF}}(t,0)$ is applied to the system operators or the system state. The HP in the IF has time-independent states and time-dependent operators:

$$\rho(t) = \rho(0); \qquad \hat{A}(t) = \hat{U}_{\mathrm{IF}}^{\dagger}(t,0)\hat{A}(0)\hat{U}_{\mathrm{IF}}(t,0). \tag{A.29}$$

The SP in the IF has time-independent states and time-dependent operators:

$$\rho(t) = \hat{U}_{\mathrm{IF}}(t,0)\rho(0)\hat{U}_{\mathrm{IF}}^{\dagger}(t,0); \qquad \hat{A}(t) = \hat{A}(0). \tag{A.30}$$

Thus the SP state in the IF is the same as the IP state (as usually defined). But the SP operators in the IF are *not* the same as the IP operators, which are evolved by $\hat{U}_0(t,0)$ as in Eq. (A.28).

We make frequent use of the interaction frame in this book, so it is necessary for the reader to understand the distinctions explained above. In fact, because we use the interaction frame so often, we frequently omit the IF subscript, after warning the reader that we are working in the interaction frame. Thus the reader must be very vigilant, since we often use the terms 'Heisenberg picture' and 'Schrödinger picture' with the phrase 'in the interaction frame' understood.

A.2 Multipartite systems and entanglement

A.2.1 Multipartite systems

Nothing is more important in quantum mechanics than understanding how to describe the state of a large system composed of subsystems. For example, in the context of measurement, we need to be able to describe the composite system composed of the

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system and the apparatus by which it is measured. The states of composite systems in quantum mechanics are described using the *tensor product*.

Consider two systems A and B prepared in the states $|\psi_{\mathrm{A}}\rangle$ and $|\psi_{\mathrm{B}}\rangle$, respectively. Let the dimension of the Hilbert space for systems A and B be D_{A} and D_{B}, respectively. The state of the total system is the tensor product state $|\Psi\rangle = |\psi_{\mathrm{A}}\rangle \otimes |\psi_{\mathrm{B}}\rangle$. More specifically, if we write the state of each component in an orthonormal basis $|\psi_{\mathrm{A}}\rangle = \sum_{j=0}^{D_{\mathrm{A}}-1} a_j |\phi_j^{\mathrm{A}}\rangle$, $|\psi_{\mathrm{B}}\rangle = \sum_{k=0}^{D_{\mathrm{B}}-1} b_k |\phi_k^{\mathrm{B}}\rangle$, then the state of the total system is

$$|\Psi\rangle = \sum_{j=0}^{D_{\mathrm{A}}-1} \sum_{k=0}^{D_{\mathrm{B}}-1} a_j b_k \big(|\phi_j\rangle_{\mathrm{A}} \otimes |\phi_k\rangle_{\mathrm{B}}\big). \tag{A.31}$$

Note that the dimension of the Hilbert space of the composite system C is $D_{\mathrm{C}} = D_{\mathrm{A}} \times D_{\mathrm{B}}$. We can define a composite basis $|\Phi_{l(k,j)}\rangle_{\mathrm{C}} = |\phi_j\rangle_{\mathrm{A}} \otimes |\phi_k\rangle_{\mathrm{B}}$, where $l(k, j)$ is a new index for the composite system. For example, we could have $l = k \times D_{\mathrm{A}} + j$. Then an arbitrary pure state of C can be written as

$$|\Psi\rangle_{\mathrm{C}} = \sum_{l=0}^{D_{\mathrm{C}}-1} c_l |\Phi_l\rangle_{\mathrm{C}}. \tag{A.32}$$

This is a vector in the compound Hilbert space $\mathbb{H}_{\mathrm{C}} = \mathbb{H}_{\mathrm{A}} \otimes \mathbb{H}_{\mathrm{B}}$. Similarly, an arbitrary mixed state for C is represented by a state matrix acting on the D_{C}-dimensional tensor-product Hilbert space.

If we have n component systems, each of dimension D, the dimension of the total system is D^n, which is exponential in n. The dimension of the Hilbert space for many-body systems is *very* big! It is worth comparing this exponential growth of Hilbert-space dimension in multi-component quantum systems with the description of multi-component classical systems. In classical mechanics, a state of complete knowledge of a single particle in three dimensions is specified by six numbers (a 3-vector each for the position and momentum). For two particles, 12 numbers are needed, and so on. That is, the size of the description increases *linearly*, not exponentially, with the number of subsystems. However, this quantum–classical difference is not present for the case of states of incomplete knowledge. For a single particle these are defined classically as a probability distribution on the configuration space (which here is the phase space) $\mathbb{R}^6$. In general this requires an infinite amount of data to represent, but this can be made finite by restricting the particle to a finite phase-space volume and introducing a minimum resolution to the description. Since the dimensionality of the phase-space increases linearly (as $6n$) with the number of particles n, the amount of data required grows exponentially, just as in the quantum case. This is an example of how quantum states are like classical states of incomplete knowledge – see also Section 1.2.1.

A.2.2 Entanglement

In Section A.1.2 we introduced the state matrix by postulating a classical source of uncertainty (in the preparation procedure). In the context of compound quantum systems, mixedness arises naturally within quantum mechanics itself. This is because of the fundamental feature of quantum mechanics termed *entanglement* by Schrödinger in 1935 [Sch35b]. Entanglement means that, even if the combined state of two systems is pure, the state of either of the subsystems need not be pure. This means that, in contrast to classical systems, maximal knowledge of the whole does not imply maximal knowledge of the

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parts. Formally, we say that the joint pure state need not factorize. That is, there exist states $|\Psi_{AB}\rangle \in \mathbb{H}_{AB} \equiv \mathbb{H}_A \otimes \mathbb{H}_B$ such that

$$|\Psi_{AB}\rangle \neq |\psi_A\rangle|\psi_B\rangle, \tag{A.33}$$

where $|\psi_A\rangle \in \mathbb{H}_A$ and $|\psi_B\rangle \in \mathbb{H}_B$. Note that we are omitting the tensor-product symbols for kets, as will be done when confusion is not likely to arise.

If we were to calculate the mean of an operator $\hat{\Lambda}_A$, operating on states in $\mathbb{H}_A$, then we would use the procedure

$$\begin{aligned}\langle\Lambda_A\rangle &= \langle\Psi_{AB}|(\hat{\Lambda}_A \otimes \hat{1}_B)|\Psi_{AB}\rangle \\ &= \sum_j \langle\Psi_{AB}|\phi_j^B\rangle\hat{\Lambda}_A\langle\phi_j^B|\Psi_{AB}\rangle = \sum_j \langle\tilde{\psi}_j^A|\hat{\Lambda}_A|\tilde{\psi}_j^A\rangle,\end{aligned} \tag{A.34}$$

where $|\tilde{\psi}_j^A\rangle$ is the unnormalized state $\langle\phi_j^B|\Psi_{AB}\rangle$. Using the fact that $\langle\psi|\hat{\Lambda}|\psi\rangle = \mathrm{Tr}\big[|\psi\rangle\langle\psi|\hat{\Lambda}\big]$, we get

$$\langle\Lambda_A\rangle = \mathrm{Tr}\left[\rho_A\hat{\Lambda}_A\right], \tag{A.35}$$

where

$$\rho_A = \sum_j \langle\phi_j^B|\Psi_{AB}\rangle\langle\Psi_{AB}|\phi_j^B\rangle \equiv \mathrm{Tr}_B[|\Psi_{AB}\rangle\langle\Psi_{AB}|] \tag{A.36}$$

is called the *reduced* state matrix for system A. The operation Tr_B is called the *partial trace* over system B.

It should be noted that the result in Eq. (A.36) also has a converse, namely that any state matrix ρ_A can be constructed as the reduced state of a (non-unique) pure state $|\Psi_{AB}\rangle$ in a larger Hilbert space. This is sometimes called a *purification* of the state matrix ρ_A, and is an example of the Gelfand–Naimark–Segal theorem [Con90].

Exercise A.9 *Construct a $|\Psi_{AB}\rangle$ that is a purification of ρ_A, given that the latter has the preparation procedure $\{\wp_j, |\psi_j\rangle\}$.*

For a bipartite system in a pure state, the entropy of one subsystem is a good measure of the degree of entanglement [NC00]. In particular, the entropy of each subsystem is the same. Note that the von Neumann entropy is *not* an extensive quantity, as is assumed in thermodynamics. As the above analysis shows, the entropy of the subsystems may be positive while the entropy of the combined system is zero. For systems with more than two parts, or for systems in mixed states, quantifying the entanglement is a far more difficult exercise, with many subtleties and as-yet unresolved issues.

The equality of the entropies of the subsystems of a pure bipartite system is known as the Araki–Lieb identity. It follows from an even stronger result: for a pure compound system, the eigenvalues of the reduced states of the subsystems are equal. This can be proven as follows. Let $\{|\phi_\lambda^A\rangle\}$ be the eigenstates of ρ_A:

$$\rho_A|\phi_\lambda^A\rangle = \wp_\lambda|\phi_\lambda^A\rangle. \tag{A.37}$$

Since these form an orthonormal set (see Box 1.1) we can write the state of the compound system using this basis for system A as

$$|\Psi_{AB}\rangle = \sum_\lambda \sqrt{\wp_\lambda}\,|\phi_\lambda^A\rangle|\phi_\lambda^B\rangle, \tag{A.38}$$

where $|\phi_\lambda^B\rangle \equiv \langle\phi_\lambda^A|\Psi_{AB}\rangle/\sqrt{\wp_\lambda}$.

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Exercise A.10 *From this definition of* $|\phi_\lambda^{\mathrm{B}}\rangle$*, show that* $\{|\phi_\lambda^{\mathrm{B}}\rangle\}$ *forms an orthonormal set, and furthermore that*

$$\rho_{\mathrm{B}}|\phi_\lambda^{\mathrm{B}}\rangle = \wp_\lambda|\phi_\lambda^{\mathrm{B}}\rangle. \tag{A.39}$$

Thus the eigenvalues of the reduced states of the two subsystems are equal. The decomposition in Eq. (A.38), using the eigenstates of the reduced states, is known as the Schmidt decomposition.

Note that the orthonormal set $\{|\phi_\lambda^{\mathrm{B}}\rangle\}$ need not be a complete basis for system B, since the dimension of B may be greater than the dimension of A. If the dimension of B is *less* than the dimension of A, then it also follows that the *rank* of ρ_{A} (that is, the number of *non-zero* eigenvalues it has) is limited to the dimensionality of B. Clearly, for a purification of ρ_{A} (as defined above), the dimensionality of B can be as low as the rank of ρ_{A}, but no lower.

A.3 Position and momentum

A.3.1 Position

Consider an operator $\hat{Q}$ having the real line as its spectrum. This could represent the position of a particle, for example. Because of its continuous spectrum, the eigenstates $|q\rangle$ of $\hat{Q}$ are not normalizable. That is, it is not possible to have $\langle q|q\rangle = 1$. Rather, we use *improper states*, normalized such that

$$\int_{-\infty}^{\infty} \mathrm{d}q|q\rangle\langle q| = \hat{1}. \tag{A.40}$$

Squaring the above equation implies that the normalization for these states is

$$\langle q|q'\rangle = \delta(q - q'). \tag{A.41}$$

The position operator is written as

$$\hat{Q} = \int \mathrm{d}q|q\rangle q\langle q|. \tag{A.42}$$

Here we are using the convention that the limits of integration are $-\infty$ to ∞ unless indicated otherwise.

A pure quantum state $|\psi\rangle$ in the position representation is a function of q,

$$\psi(q) = \langle q|\psi\rangle, \tag{A.43}$$

commonly called the *wavefunction*. The probability density for finding the particle at position q is $|\psi(q)|^2$, and this integrates to unity. The state $|\psi\rangle$ is recovered from the wavefunction as follows:

$$|\psi\rangle = \int \mathrm{d}q|q\rangle\langle q|\psi\rangle = \int \mathrm{d}q\ \psi(q)|q\rangle. \tag{A.44}$$

It is worth remarking more about the nature of the continuum in quantum mechanics. The probability interpretation of the function $\psi(q)$ requires that it belong to the set $L^{(2)}(\mathbb{R})$. That is, the integral (technically, a Lebesgue integral) $\int |\psi(q)|^2\,\mathrm{d}q$ must be finite, so that it can be set equal to unity for a normalized wavefunction. Although the space of $L^{(2)}(\mathbb{R})$ functions is infinite-dimensional, it is a countable infinity. That is, the basis states for the Hilbert space $\mathbb{H} = L^{(2)}(\mathbb{R})$ can be labelled by integers; an example basis is the set

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of harmonic-oscillator eigenstates discussed in Section A.4.1 below. The apparent continuum of the position states $\{|q\rangle\}$ (or the momentum states $\{|p\rangle\}$ defined below) does not contradict this: these 'states' are not normalizable and so are not actually in the Hilbert space. They exist as limits of true states, but the limit lies outside $\mathbb{H}$.

A.3.2 Momentum

It turns out that, if $\hat{Q}$ does represent the position of a particle, then its momentum is represented by another operator with the real line as its spectrum, $\hat{P}$. Using $\hbar = 1$, the eigenstates for $\hat{P}$ are related to those for $\hat{Q}$ by

$$\langle q|p\rangle = (2\pi)^{-1/2} \mathrm{e}^{\mathrm{i}pq}. \tag{A.45}$$

Here the normalization factor is chosen so that, analogously to Eqs. (A.40) and (A.41), we have

$$\int \mathrm{d}p |p\rangle\langle p| = \hat{1}, \qquad \langle p|p'\rangle = \delta(p - p'). \tag{A.46}$$

Exercise A.11 *Show Eq. (A.46), using the position representation and the result that* $\int \mathrm{d}y\, \mathrm{e}^{\mathrm{i}yx} = 2\pi\delta(x)$.

The momentum-representation wavefunction is thus simply the Fourier transform of the position-representation wavefunction:

$$\psi(p) = \langle p|\psi\rangle = (2\pi)^{-1/2} \int \mathrm{d}q\, \mathrm{e}^{-\mathrm{i}pq} \psi(q). \tag{A.47}$$

From the above it is easy to show that in the position representation $\hat{P}$ acts on a wavefunction identically to the differential operator $-\mathrm{i}\,\partial/\partial q$. First, in the momentum representation,

$$\hat{P} = \int \mathrm{d}p |p\rangle p \langle p|. \tag{A.48}$$

Thus,

$$\langle q|\hat{P}|\psi\rangle = \int \mathrm{d}p \int \mathrm{d}q' \langle q|p\rangle p \langle p|q'\rangle\langle q'|\psi\rangle \tag{A.49}$$

$$= (2\pi)^{-1} \int \mathrm{d}p \int \mathrm{d}q'\, p \mathrm{e}^{\mathrm{i}p(q-q')} \psi(q'). \tag{A.50}$$

Now $p\mathrm{e}^{\mathrm{i}p(q-q')} = \mathrm{i}\,\partial \mathrm{e}^{\mathrm{i}p(q-q')}/\partial q'$, so, using integration by parts and the fact (required by normalization) that $\psi(q)$ vanishes at $\pm\infty$, we obtain

$$\langle q|\hat{P}|\psi\rangle = -\mathrm{i}(2\pi)^{-1} \int \mathrm{d}p \int \mathrm{d}q'\, \mathrm{e}^{\mathrm{i}p(q-q')} \frac{\partial}{\partial q'} \psi(q') \tag{A.51}$$

$$= -\mathrm{i} \frac{\partial}{\partial q} \psi(q). \tag{A.52}$$

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It is now easy to find the commutator between $\hat{Q}$ and $\hat{P}$:

$$\langle q|[\hat{Q},\hat{P}]|\psi\rangle = \langle q|[\hat{Q},\hat{P}]\int \mathrm{d}q'\,\psi(q')|q'\rangle \tag{A.53}$$

$$= q(-\mathrm{i})\frac{\partial}{\partial q}\psi(q) - (-\mathrm{i})\frac{\partial}{\partial q}q\psi(q) \tag{A.54}$$

$$= \mathrm{i}\psi(q) = \mathrm{i}\langle q|\psi\rangle. \tag{A.55}$$

Now $\psi(q)$ here is an arbitrary function, apart from the assumption of differentiability and vanishing at $\pm\infty$. Thus it must be that

$$[\hat{Q},\hat{P}] = \mathrm{i}. \tag{A.56}$$

The fact that the commutator here is a c-number makes this an example of a *canonical commutation relation.*

A.3.3 Minimum-uncertainty states

From the above canonical commutation relation it follows (see Exercise A.3) that the variances in Q and P must satisfy

$$\left\langle(\Delta P)^2\right\rangle\left\langle(\Delta Q)^2\right\rangle \geq 1/4. \tag{A.57}$$

(Remember that we have set $\hbar = 1$.) The states which saturate this are known as minimum-uncertainty states (MUSs). It can be shown that these are Gaussian pure states. By this we mean that they are states with a Gaussian wavefunction. For a MUS, they are parameterized by three real numbers. Below, we take these to be q_0, p_0 and σ.

The position probability amplitude (i.e. wavefunction) for a MUS takes the form

$$\psi(q) = (\pi\sigma^2)^{-1/4}\exp\left[+\mathrm{i}p_0(q-q_0) - (q-q_0)^2/(2\sigma^2)\right]. \tag{A.58}$$

Here we have chosen the overall phase factor to give $\psi(q)$ a real maximum at $q = q_0$. It is then easily verified that the moments for Q are

$$\langle Q\rangle = q_0, \tag{A.59}$$

$$\langle(\Delta Q)^2\rangle = \sigma^2/2. \tag{A.60}$$

Note that the variance does not equal σ^2, as one might expect from Eq. (A.58), because $\wp(q) = |\psi(q)|^2$.

The Fourier transform of a Gaussian is also Gaussian, and in the momentum representation

$$\psi(p) = (\pi/\sigma^2)^{-1/4}\exp\left[-\mathrm{i}q_0 p - (p-p_0)^2\sigma^2/2\right]. \tag{A.61}$$

From this it is easy to show that

$$\langle P\rangle = p_0, \tag{A.62}$$

$$\langle(\Delta P)^2\rangle = 1/(2\sigma^2). \tag{A.63}$$

The saturation of the Heisenberg bound (A.57) follows.

Exercise A.12 *Verify Eqs. (A.59)–(A.63).*

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A.4 The harmonic oscillator

So far there is nothing that sets a natural length (or, consequently, momentum) scale for the system. The simplest dynamics which does so is that generated by the harmonic oscillator Hamiltonian

$$\hat{H} = \frac{\hat{P}^2}{2m} + \frac{m\omega^2 \hat{Q}^2}{2}. \tag{A.64}$$

Here m is the mass of the particle and ω is the oscillator frequency. This Hamiltonian applies to any mode of harmonic oscillation, such as a mode of a sound wave in a condensed-matter system, or a mode of the electromagnetic field. In the latter case, $\hat{Q}$ is proportional to the magnetic field and $\hat{P}$ to the electric field.

Classically the harmonic oscillator has no characteristic length scale, but quantum mechanically it does, namely

$$\sigma = \sqrt{\hbar/(m\omega)}, \tag{A.65}$$

where we have temporarily restored $\hbar$ to make its role apparent. If we define the (non-Hermitian) operator

$$\hat{a} = \frac{1}{\sqrt{2}}\left(\frac{\hat{Q}}{\sigma} + \mathrm{i}\frac{\sigma \hat{P}}{\hbar}\right) \tag{A.66}$$

then we can rewrite the Hamiltonian as

$$H = \hbar\omega(\hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger)/2 = \hbar\omega(\hat{a}^\dagger\hat{a} + \tfrac{1}{2}). \tag{A.67}$$

Now, from the commutation relations of $\hat{Q}$ and $\hat{P}$ we can show that

$$[\hat{a}, \hat{a}^\dagger] = 1. \tag{A.68}$$

Also, we can show that the state $|\psi_0\rangle$ with wavefunction

$$\psi_0(q) = \langle q|\psi_0\rangle \propto \exp[-q^2/(2\sigma^2)] \tag{A.69}$$

is an eigenstate of $\hat{a}$ with eigenvalue 0.

Exercise A.13 *Show this using the position representation of $\hat{P}$ as $-\mathrm{i}\hbar\,\partial/\partial q$.*

Thus it is also an eigenstate of the Hamiltonian (A.67), with eigenvalue $\hbar\omega/2$. Since $\hat{a}^\dagger\hat{a}$ is obviously a positive semi-definite operator, this is the lowest eigenvalue of the Hamiltonian. That is, we have shown that the quantum harmonic oscillator has a *ground state* that is a minimum-uncertainty state with $q_0 = p_0 = 0$ and a characteristic length σ given by Eq. (A.65).

A.4.1 Number states

From the above it is easy to show that the eigenvalues of $\hat{a}^\dagger\hat{a}$ are the non-negative integers, as follows. From the commutation relations (A.68) it follows that (for integer k)

$$[\hat{a}^\dagger\hat{a}, (\hat{a}^\dagger)^k] = \hat{a}^\dagger[\hat{a}, (\hat{a}^\dagger)^k] = k(\hat{a}^\dagger)^k. \tag{A.70}$$

Exercise A.14 *Show this.*
Hint: *Start by showing it for $k = 1$ and $k = 2$ and then find a proof by induction.*

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Then, if we define an unnormalized state $|\psi_n\rangle = (\hat{a}^\dagger)^n|\psi_0\rangle$ we can easily show that

$$(\hat{a}^\dagger\hat{a})|\psi_n\rangle = (\hat{a}^\dagger\hat{a})(\hat{a}^\dagger)^n|\psi_0\rangle = \left[n(\hat{a}^\dagger)^n + (\hat{a}^\dagger)^n(\hat{a}^\dagger\hat{a})\right]|\psi_0\rangle$$
$$= n(\hat{a}^\dagger)^n|\psi_0\rangle = n|\psi_n\rangle, \tag{A.71}$$

which establishes the result and identifies the eigenstates.

Thus we have derived the eigenvalues of the harmonic oscillator as $\hbar\omega\left(n + \frac{1}{2}\right)$. The corresponding unnormalized eigenstates are $|\psi_n\rangle$, which we denote $|n\rangle$ when normalized. If the Hamiltonian (A.64) refers to a particle, these are states with an integer number of elementary excitations of the vibration of the particle. They are therefore sometimes called *vibron* number states, that is, states with a definite number of vibrons. If the harmonic oscillation is that of a sound wave, then these states are called *phonon* number states. If the oscillator is a mode of the electromagnetic field, they are called *photon* number states. Especially in the last case, the ground state $|0\rangle$ is often called the vacuum state.

The operator $\hat{N} = \hat{a}^\dagger\hat{a}$ is called the *number operator*. Because $\hat{a}^\dagger$ raises the number of excitations by one, with

$$|n\rangle \propto (\hat{a}^\dagger)^n|0\rangle, \tag{A.72}$$

it is called the creation operator. Similarly, $\hat{a}$ lowers it by one, and is called the annihilation operator. To find the constants of proportionality, we must require that the number states be normalized, so that

$$\langle n|m\rangle = \delta_{nm}. \tag{A.73}$$

Now, since $|n\rangle$ is an eigenstate of $a^\dagger a$ with eigenvalue n,

$$\langle n|\hat{a}^\dagger\hat{a}|n\rangle = n\langle n|n\rangle = n. \tag{A.74}$$

However, we also have

$$\langle n|\hat{a}^\dagger\hat{a}|n\rangle = \langle\psi|\psi\rangle, \tag{A.75}$$

where $|\psi\rangle = \hat{a}|n\rangle \propto |n-1\rangle$. Thus the constant of proportionality must be such that

$$|\psi\rangle = \hat{a}|n\rangle = \mathrm{e}^{\mathrm{i}\phi}\sqrt{n}|n-1\rangle \tag{A.76}$$

for some phase ϕ. We choose the convention that $\phi = 0$, so that

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle. \tag{A.77}$$

Similarly, it can be shown that

$$\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle. \tag{A.78}$$

Exercise A.15 *Show this, and show that the above two relations are consistent with* $|n\rangle$ *being an eigenstate of* $\hat{a}^\dagger\hat{a}$. *Show also that the normalized number state is given by* $|n\rangle = (n!)^{-1/2}(\hat{a}^\dagger)^n|0\rangle$.

Note that $\hat{a}$ acting on the vacuum state $|0\rangle$ produces nothing, a null state.

A.4.2 Coherent states

No matter how large n is, a number state $|n\rangle$ never approaches the classical limit of an oscillating particle (or oscillating field amplitude). That is because for a system in a number state the average values of Q and P are always zero.

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Exercise A.16 *Show this.*

For this reason, it is useful to consider a state for which there is a classical limit, the *coherent* state. This state is defined as an eigenstate of the annihilation operator

$$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle, \tag{A.79}$$

where α is a complex number (because $\hat{a}$ is not an Hermitian operator). There are no such eigenstates of the creation operator $\hat{a}^\dagger$.

Exercise A.17 *Show this.*
Hint: *Assume that there exist states $|\beta\rangle$ such that $\hat{a}^\dagger|\beta\rangle = \beta|\beta\rangle$ and consider the inner product $\langle n|(\hat{a}^\dagger)^{n+1}|\beta\rangle$. Hence show that the inner product of $|\beta\rangle$ with any number state is zero.*

It is easy to find an expression for $|\alpha\rangle$ in terms of the number states as follows. In general we have

$$|\alpha\rangle = \sum_{n=0}^{\infty} c_n|n\rangle. \tag{A.80}$$

Since $\hat{a}|\alpha\rangle = \alpha|\alpha\rangle$ we get

$$\sum_{n=0}^{\infty} \sqrt{n}c_n|n-1\rangle = \sum_{n=0}^{\infty} \alpha c_n|n\rangle. \tag{A.81}$$

By equating the coefficients of the number states on both sides we get the recursion relation

$$c_{n+1} = \frac{\alpha}{\sqrt{n+1}}c_n, \tag{A.82}$$

so that $c_n = (\alpha^n/\sqrt{n!})c_0$. On choosing c_0 real and normalizing the state, we get

$$|\alpha\rangle = \exp\left(-|\alpha|^2/2\right) \sum_n \frac{\alpha^n}{\sqrt{n!}}|n\rangle. \tag{A.83}$$

The state $|\alpha := 0\rangle$ is the same state as the state $|n := 0\rangle$. For α finite the coherent state has a non-zero mean photon number:

$$\langle\alpha|\hat{a}^\dagger\hat{a}|\alpha\rangle = \left(\langle\alpha|\alpha^*\right)(\alpha|\alpha\rangle) = |\alpha|^2. \tag{A.84}$$

The number distribution (the probability of measuring a certain excitation number) for a coherent state is a *Poissonian* distribution of mean $|\alpha|^2$:

$$\wp_n = |\langle n|\alpha\rangle|^2 = \mathrm{e}^{-|\alpha|^2}\frac{\left(|\alpha|^2\right)^n}{n!}. \tag{A.85}$$

This distribution has the property that the variance is equal to the mean. That is,

$$\left\langle(\hat{a}^\dagger\hat{a})^2\right\rangle - \left\langle\hat{a}^\dagger\hat{a}\right\rangle^2 = |\alpha|^2. \tag{A.86}$$

Exercise A.18 *Verify this, either from the distribution (A.85) or directly from the coherent state using the commutation relations for $\hat{a}$ and $\hat{a}^\dagger$.*

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Setting $\hbar = 1$, it is simple to show that

$$\langle\alpha|\hat{Q}|\alpha\rangle = \sqrt{2}\sigma\,\mathrm{Re}[\alpha], \tag{A.87}$$

$$\langle\alpha|\hat{P}|\alpha\rangle = (\sqrt{2}/\sigma)\mathrm{Im}[\alpha], \tag{A.88}$$

$$\langle\alpha|(\Delta\hat{Q})^2|\alpha\rangle = \sigma^2/2, \tag{A.89}$$

$$\langle\alpha|(\Delta\hat{P})^2|\alpha\rangle = 1/(2\sigma^2), \tag{A.90}$$

$$\langle\alpha|\Delta\hat{Q}\,\Delta\hat{P} + \Delta\hat{P}\,\Delta\hat{Q}|\alpha\rangle = 0. \tag{A.91}$$

That is, a coherent state is a minimum-uncertainty state, as defined in Section A.3.3.

Because $\hat{a}$ is not Hermitian, the coherent states do not form an orthonormal set. In fact it can be shown that

$$\langle\beta|\alpha\rangle = \mathrm{e}^{\beta^*\alpha - (|\alpha|^2 + |\beta|^2)/2}, \tag{A.92}$$

from which it follows that $|\langle\beta|\alpha\rangle|^2 = \mathrm{e}^{-|\alpha-\beta|^2}$. If α and β are very different (as they would be if they represent two macroscopically distinct fields) then the two coherent states are very nearly orthogonal. Another consequence of their non-orthogonality is that the coherent states form an *overcomplete* basis. Whereas for number states we have

$$\sum_n |n\rangle\langle n| = \hat{1}, \tag{A.93}$$

the identity, for coherent states we have

$$\int \mathrm{d}^2\alpha |\alpha\rangle\langle\alpha| = \pi\hat{1}. \tag{A.94}$$

This has applications in defining the trace, for example

$$\mathrm{Tr}[\rho] = \frac{1}{\pi}\int \mathrm{d}^2\alpha \langle\alpha|\rho|\alpha\rangle. \tag{A.95}$$

Exercise A.19 *Show Eq. (A.94) using the expansion (A.83).*
Hint: *Write* $\alpha = r\mathrm{e}^{\mathrm{i}\phi}$ *so that* $\mathrm{d}^2\alpha = r\,\mathrm{d}r\,\mathrm{d}\phi$. *The result* $n! = \int_0^\infty \mathrm{d}x\, x^n \mathrm{e}^{-x}$ *may be useful.*

Unlike number states, coherent states are not eigenstates of the Hamiltonian. However, they have the nice property that they remain as coherent states under evolution generated by the harmonic-oscillator Hamiltonian

$$\hat{H} = \omega\hat{a}^\dagger\hat{a}. \tag{A.96}$$

Here we have dropped the $1/2$ from the Hamiltonian (A.67) since it has no physical consequences (at least outside general relativity). The amplitude $|\alpha|$ of the states remains the same; only the phase changes at rate ω (as expected):

$$\exp(-\mathrm{i}\hat{H}t)|\alpha\rangle = |\mathrm{e}^{-\mathrm{i}\omega t}\alpha\rangle. \tag{A.97}$$

Exercise A.20 *Show this, using Eq. (A.83).*

This form-invariance under the harmonic-oscillator evolution is why they are called coherent states.

Coherent states can be generated from the vacuum state as follows:

$$|\alpha\rangle = \hat{D}(\alpha)|0\rangle, \tag{A.98}$$

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where

$$\hat{D}(\alpha) = \mathrm{e}^{\alpha\hat{a}^\dagger - \alpha^*\hat{a}} = \mathrm{e}^{-\mathrm{i}(\mathrm{i}\alpha\hat{a}^\dagger - \mathrm{i}\alpha^*\hat{a})} \tag{A.99}$$

is called the displacement operator. This is easiest to see as follows. First, note that if we define the family of operators $\hat{O}_\mu = \hat{U}_\mu^\dagger \hat{O}_0 \hat{U}_\mu$, where $\hat{U}_\mu = \mathrm{e}^{(\alpha\hat{a}^\dagger - \alpha^*\hat{a})\mu}$, then these are solutions to the equation

$$\frac{\mathrm{d}}{\mathrm{d}\mu}\hat{O}_\mu = -[\alpha\hat{a}^\dagger - \alpha^*\hat{a}, \hat{O}_\mu]. \tag{A.100}$$

Exercise A.21 *Show this, by analogy with the Heisenberg equations of motion.*

Now, applying this to $\hat{O}_0 = \hat{a}$, we see that $\hat{O}_\mu = \hat{a} + \mu\alpha$ is a solution to Eq. (A.100). Then, noting that $\hat{D}(\alpha) = \hat{U}_1 = \hat{D}^\dagger(-\alpha)$, we have

$$\hat{a}\hat{D}(\alpha)|0\rangle = \hat{D}(\alpha)\hat{D}^\dagger(\alpha)\hat{a}\hat{D}(\alpha)|0\rangle = \hat{D}(\alpha)(\hat{a} + \alpha)|0\rangle = \alpha\hat{D}(\alpha)|0\rangle, \tag{A.101}$$

which proves the above result.

A.4.3 Squeezed states

Because the harmonic-oscillator Hamiltonian picks out a particular class of minimum-uncertainty states (the coherent states), the other minimum-uncertainty states are given a special name in this situation: the squeezed states. In fact, any Gaussian pure state other than a coherent state is called a squeezed state. Whereas a coherent state requires one complex parameter α to specify, a general squeezed state requires two additional real parameters:

$$|\alpha, r, \phi\rangle = \hat{D}(\alpha)|r, \phi\rangle, \tag{A.102}$$

where

$$|r, \phi\rangle = \exp\left[r\left(\mathrm{e}^{-2\mathrm{i}\phi}\hat{a}^2 - \mathrm{e}^{2\mathrm{i}\phi}\hat{a}^{\dagger 2}\right)/2\right]|0\rangle \tag{A.103}$$

is known as a squeezed vacuum. This is an appropriate name since it is in fact a zero-amplitude coherent state for rotated and rescaled canonical coordinates, $\hat{Q}'$ and $\hat{P}'$, defined by

$$\hat{Q} + \mathrm{i}\hat{P} = (\hat{Q}'\mathrm{e}^{r} + \mathrm{i}\hat{P}'\mathrm{e}^{-r})\mathrm{e}^{\mathrm{i}\phi}. \tag{A.104}$$

For example, if $\phi = 0$ then $\hat{P} = \mathrm{e}^{-r}\hat{P}'$, so the variance of P is smaller by a factor of e^{-2r} than that of a coherent state. By contrast, $\hat{Q} = \mathrm{e}^{r}\hat{Q}'$, so the variance of Q is e^{2r} times larger than that of a coherent state. That is, the reduction in the variance of one coordinate *squeezes* the uncertainty into the conjugate coordinate. The term squeezed state is often applied more broadly, to any state (pure or mixed, Gaussian or not) of a harmonic oscillator in which the uncertainty in one coordinate is below that of the vacuum state.

A.5 Quasiprobability distributions

It is often convenient to represent quantum states as quantum probability distributions, or quasiprobability distributions, over non-commuting observables. Here we consider the

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three most commonly used distributions, called the P, Q and W distributions (or functions).

A.5.1 Normal order and the P function

Once an annihilation operator has been defined, *normal ordering* can be defined. A normally ordered operator expression is one in which all annihilation operators appear to the right of all creation operators. For example, $\hat{A} = (\hat{a}^\dagger \hat{a})^2$ is not a normally ordered operator expression, but $\hat{A} = \hat{a}^\dagger \hat{a}^\dagger \hat{a}\hat{a} + \hat{a}^\dagger \hat{a}$ *is* a normally ordered expression. Note that this example shows that it does not make sense to speak of a 'normally ordered operator' (although this is common parlance), since it is the *same* operator being represented here, in one case by a normally ordered expression and in the other by a non-normally ordered expression. One advantage of normal ordering is that one can see immediately whether any term will give zero when acting on a vacuum state by seeing whether it has at least one annihilation operator.

Classically, the c-number analogues of $\hat{a}$ and $\hat{a}^\dagger$, which we can denote α and α^*, commute. This means that, regardless of the ordering of an expression $f(\alpha, \alpha^*)$, we have

$$\left\langle f(\alpha, \alpha^*) \right\rangle = \int \mathrm{d}^2\alpha \; P(\alpha, \alpha^*) f(\alpha, \alpha^*), \tag{A.105}$$

where $P(\alpha, \alpha^*)$ is a probability distribution over phase-space.[1] Quantum mechanically, we do have to worry about ordering, but we could ask the following: for a given ρ, is there a distribution P such that

$$\mathrm{Tr}[\rho f_n(\hat{a}, \hat{a}^\dagger)] = \int \mathrm{d}^2\alpha \; P(\alpha, \alpha^*) f_n(\alpha, \alpha^*), \tag{A.106}$$

where f_n is a normally ordered expression? The answer is yes, but in general P is an extremely singular function (i.e. more singular than a δ-function). The relation between the P function (as it is called) and ρ is

$$\rho = \int \mathrm{d}^2\alpha \; P(\alpha, \alpha^*) |\alpha\rangle\langle\alpha|. \tag{A.107}$$

Thus, if P is only as singular as a δ-function, then ρ is a mixture of coherent states.

Exercise A.22 *Assuming a non-singular P function, verify Eq. (A.106) from Eq. (A.107).*

A.5.2 Antinormal order and the Q function

Antinormal ordering is, as its name implies, the opposite to normal ordering. For example, $\hat{A} = \hat{a}\hat{a}\hat{a}^\dagger\hat{a}^\dagger - 3\hat{a}\hat{a}^\dagger + 1$ is an antinormally ordered operator expression for the operator $\hat{A}$ defined above. As for normal ordering, one can ask the question, for a given ρ, is there a distribution Q such that

$$\mathrm{Tr}[\rho f_a(\hat{a}, \hat{a}^\dagger)] = \int \mathrm{d}^2\alpha \; Q(\alpha, \alpha^*) f_a(\alpha, \alpha^*), \tag{A.108}$$

[1] We write, for example, $P(\alpha, \alpha^*)$ rather than $P(\alpha)$, to avoid implying (wrongly) that these functions are analytical functions in the complex plane.

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where f_a is an *antinormally* ordered expression? Again the answer is yes. Moreover, the Q function (as it is called) is always smooth and positive, and is given by

$$Q(\alpha, \alpha^*) = \pi^{-1}\langle\alpha|\rho|\alpha\rangle. \tag{A.109}$$

Exercise A.23 *From this definition, verify Eq. (A.108).*

A.5.3 Symmetric order and the Wigner function

A final type of ordering commonly used is symmetric ordering. This can be defined independently of an annihilation operator, as an expression that is symmetric in $\hat{a}$ and $\hat{a}^\dagger$ is also symmetric in position $\hat{Q}$ and momentum $\hat{P}$. A symmetric operator expression is one in which every possible ordering is equally weighted. Using the same example as previously, a symmetric expression is

$$\hat{A} = \frac{1}{6}\big[\hat{a}^\dagger\hat{a}^\dagger\hat{a}\hat{a} + \hat{a}^\dagger\hat{a}\hat{a}^\dagger\hat{a} + \hat{a}^\dagger\hat{a}\hat{a}\hat{a}^\dagger + \hat{a}\hat{a}^\dagger\hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger\hat{a}\hat{a}^\dagger + \hat{a}\hat{a}\hat{a}^\dagger\hat{a}^\dagger\big]$$
$$- \frac{1}{2}\big[\hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger\big]. \tag{A.110}$$

We can ask the same question as in the preceding subsections, namely is there a distribution function W such that

$$\mathrm{Tr}[\rho f_s(\hat{a}, \hat{a}^\dagger)] = \int \mathrm{d}^2\alpha\, W(\alpha, \alpha^*) f_s(\alpha, \alpha^*), \tag{A.111}$$

where f_s is a symmetrically ordered expression? The answer again is yes, and this distribution is known as the Wigner function, because it was introduced by Wigner [Wig32]. Its relation to ρ is that

$$W(\alpha, \alpha^*) = \frac{1}{\pi^2}\int \mathrm{d}^2\omega\, \mathrm{Tr}\big[\rho\, \exp[\omega(\hat{a}^\dagger - \alpha^*) - \omega^*(\hat{a} - \alpha)]\big]. \tag{A.112}$$

The Wigner function is always a smooth function, but it can take negative values. It was originally defined by Wigner as a function of position q and momentum p. From Eq. (A.66), with $\hbar = 1$, these are related to α by

$$\alpha = \frac{1}{\sqrt{2}}\Big(\frac{q}{\sigma} + \mathrm{i}\sigma p\Big). \tag{A.113}$$

In terms of these variables (using $\omega = x - \mathrm{i}k$),

$$W(q, p) = \frac{1}{(2\pi)^2}\int \mathrm{d}k \int \mathrm{d}x\, \mathrm{Tr}\big[\rho\, \exp[\mathrm{i}k(\hat{Q} - q) + \mathrm{i}x(\hat{P} - p)]\big]. \tag{A.114}$$

Note that the characteristic length σ of the harmonic oscillator does not enter into this expression.

A particularly appealing feature of the Wigner function is that its marginal distributions are the true probability distributions. That is,

$$\int \mathrm{d}q\, W(q, p) = \wp(p) = \langle p|\rho|p\rangle, \tag{A.115}$$

$$\int \mathrm{d}p\, W(q, p) = \wp(q) = \langle q|\rho|q\rangle. \tag{A.116}$$

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Exercise A.24 *Show this.*
Hint: *Recall that* $\int \mathrm{d}q\, \mathrm{e}^{\mathrm{i}pq} = 2\pi\delta(p)$ *and that* $\delta(p - \hat{P}) = |p\rangle\langle p|$.

The Wigner function thus appears like a joint classical probability distribution, except that in many cases it is not positive definite. Indeed, of the pure states, only states with a Gaussian wavefunction $\psi(q)$ have a positive-definite Wigner function. Another appealing property of the Wigner function is that the overlap between two states is given simply by the integral of the products of their respective Wigner functions:

$$\mathrm{Tr}[\rho_1\rho_2] = 2\pi\hbar \int \mathrm{d}q \int \mathrm{d}p\, W_1(q, p)W_2(q, p). \tag{A.117}$$

Exercise A.25 *Show this.*

Finally, the Baker–Campbell–Hausdorff theorem states that, for arbitrary operators $\hat{A}$ and $\hat{B}$ satisfying $[\hat{A}, [\hat{A}, \hat{B}]] = 0$ and $[\hat{B}, [\hat{A}, \hat{B}]] = 0$,

$$\exp(\hat{A} + \hat{B}) = \exp(\hat{A})\exp(\hat{B})\exp(-\tfrac{1}{2}[\hat{A}, \hat{B}]). \tag{A.118}$$

Using this, the Wigner function can be rewritten as

$$W(q, p) = \frac{1}{(2\pi)^2} \int \mathrm{d}k \int \mathrm{d}x\, \mathrm{Tr}\Big[\rho \mathrm{e}^{\mathrm{i}k(\hat{Q}-q)}\mathrm{e}^{\mathrm{i}x(\hat{P}-p)}\mathrm{e}^{-\mathrm{i}kx/2}\Big] \tag{A.119}$$

$$= \frac{1}{(2\pi)^2} \int \mathrm{d}k \int \mathrm{d}x\, \mathrm{Tr}\Big[\rho \mathrm{e}^{\mathrm{i}x(\hat{P}-p)}\mathrm{e}^{\mathrm{i}k(\hat{Q}-q)}\mathrm{e}^{+\mathrm{i}kx/2}\Big]. \tag{A.120}$$

From this, it is easy to prove the following useful operator correspondences:

$$\hat{Q}\rho \leftrightarrow \left(q + \frac{\mathrm{i}}{2}\frac{\partial}{\partial p}\right) W(q, p), \tag{A.121}$$

$$\rho\hat{Q} \leftrightarrow \left(q - \frac{\mathrm{i}}{2}\frac{\partial}{\partial p}\right) W(q, p), \tag{A.122}$$

$$\hat{P}\rho \leftrightarrow \left(p - \frac{\mathrm{i}}{2}\frac{\partial}{\partial q}\right) W(q, p), \tag{A.123}$$

$$\rho\hat{P} \leftrightarrow \left(p + \frac{\mathrm{i}}{2}\frac{\partial}{\partial q}\right) W(q, p). \tag{A.124}$$

Exercise A.26 *Show these. This means showing, for example, that*

$$\int \mathrm{d}k \int \mathrm{d}x\, \mathrm{Tr}\Big[\mathrm{e}^{\mathrm{i}x(\hat{P}-p)}\mathrm{e}^{\mathrm{i}k(\hat{Q}-q)}\mathrm{e}^{+\mathrm{i}kx/2}\hat{Q}\rho\Big]$$

$$= \int \mathrm{d}k \int \mathrm{d}x \left(q + \frac{\mathrm{i}}{2}\frac{\partial}{\partial p}\right) \mathrm{Tr}\Big[\mathrm{e}^{\mathrm{i}x(\hat{P}-p)}\mathrm{e}^{\mathrm{i}k(\hat{Q}-q)}\mathrm{e}^{+\mathrm{i}kx/2}\rho\Big]. \tag{A.125}$$

Note that here ρ is not restricted to being a state matrix. It can be an arbitrary operator with Wigner representation $W(q, p)$, provided that the integrals converge and boundary terms can be ignored.

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