The Dirac notation in quantum optics
Rev. 4

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Foreword

This PM outlines the basics of the Dirac notation in quantum mechanics. This notation is particularly useful in quantum optics where the wave-function notation is seldom used. The PM has been used in the course "Quantum electronics with Electro Optics" and its predecessors at KTH for a number of years. In the course, the material has been presented during roughly six 45 minute lectures. The PM was also used at the "Nordic summer-school in non-linear and quantum optics" held at Hensbacka, Sweden in 1997. The PM has been updated in the summer of 2003, in 2011, and in early 2015 to reflect some of the recent developments in quantum optics, and some minor corrections have been made. The goal of the PM is to provide a concise introduction to the Dirac formalism, sufficient for the student to get to the point where he or she can analyze simple, but realistic, contemporary experiments in quantum optics.

In the PM, most assertions are left without proof. The interested reader will find the proofs in a comprehensive elementary textbook of quantum mechanics, e.g., "Quantum Mechanics" by C. Cohen-Tannoudji, B. Diu and F. Laloë, Wiley Interscience, New York, 1977.

1 State vectors

The fundamental entities in quantum mechanics are the states of objects and the associated operators. P. A. M. Dirac formulated a concise and convenient formalism for making quantum mechanical calculations and writing quantum mechanical expressions. In Dirac's notation, a (pure) quantum mechanical object can be completely described by its state vector. The state vectors come in two "flavors", bras and kets. These contain identical information and are adjoint vectors in a Hilbert space $\mathcal{H}$. The ket is written $|\psi\rangle$, where the index ψ specifies the state. The associated vector is called a bra and is written $\langle\psi|$. A state can be expanded in a linear combination of other states:

$$|\psi\rangle = \sum_n c_n |\phi_n\rangle, \tag{1}$$

where $c_n \in \mathcal{C}$ and $\mathcal{C}$ is the set of complex numbers. The state $|\psi\rangle$ is said to be in a *superposition* of the states $|\phi_n\rangle$.

The scalar product (or inner product) of two state vectors is written

$$(|\psi\rangle, |\phi\rangle) = \langle\psi|\phi\rangle. \tag{2}$$

The associated vector $\langle\psi|$ is the Hermitian conjugate of the corresponding ket. Hermitian conjugation is denoted by † and and is a linear operation. Conjugation of a scalar c, a linear operator $\hat{A}$ and a ket $|\psi\rangle$ gives c^*, $\hat{A}^\dagger$, $\langle\psi|$, respectively, where * denotes the complex conjugation. Two successive conjugations cancel, therefore the respective elements above are mutually conjugate.

When a simple product of operators and/or states is conjugated the factors are both conjugated and their mutual order is reversed, viz.

$$\langle\phi|\psi\rangle^\dagger = \langle\psi|\phi\rangle. \tag{3}$$

In this particular case, since the *scalar* product is a complex number we can simplify the expression to

$$\langle\psi|\phi\rangle = \langle\phi|\psi\rangle^*. \tag{4}$$

When products of more than two factors are conjugated, one repeatedly applies the rule above, e.g.

$$(\langle\phi|\hat{A}|\psi\rangle)^\dagger = \langle\psi|(\langle\phi|\hat{A})^\dagger = \langle\psi|\hat{A}^\dagger|\phi\rangle. \tag{5}$$

Unlike vectors in $\mathcal{R}^n$-space, overall multiplicative factors of the state vector are insignificant. Hence, $|\psi\rangle$ and $c|\psi\rangle$, where $c \in \{\mathcal{C}\backslash 0\}$, represent the same state. By convention (and to simplify the probabilistic interpretation of the state vector) normalized state vectors are used, i.e.

$$\langle\psi|\psi\rangle = 1. \tag{6}$$

Therefore every state correspond to a unique state vector (except for a trivial overall phase factor). The probability of finding the object (described by the state vector $|\psi\rangle$ in the state $|\phi_n\rangle$ is given by

$$0 \leq |\langle\psi|\phi_n\rangle|^2 \leq 1. \tag{7}$$

Two states are orthogonal if

$$\langle\psi|\phi\rangle = 0, \tag{8}$$

and are identical if

$$|\langle\psi|\phi\rangle| = 1. \tag{9}$$

Suppose all the states in the set $\{|\phi_n\rangle\}$ are orthonormal. Under certain conditions (that we will outline below) *any* state can be expressed in a superposition of these basis states. If so, the set $\{|\phi_n\rangle\}$ is a *complete* orthonormal basis. From (1) and (7) it follows that the probability of finding the object in the state $|\phi_n\rangle$ is $|c_n|^2$, i.e. the square modulus of the object-state expansion-coefficient.

2 Number states

At the beginning of this century physicists discovered that the thermal, electromagnetic emission spectrum could be explained if it was assumed that the electromagnetic field was quantized in energy units of $h\nu$, where h is Planck's constant and ν is the frequency. The observation was later supplemented by the observation of the photo-electric effect. The quantum unit of electromagnetic energy was eventually called a photon (after the Greek word *phos* = light). Since energy is an observable, it is associated with a Hermitian operator (see below) and (this is no coincidence) with a complete set of eigenstates. Since the energy of any such eigenstate can be written $h\nu(n + 1/2)$, where $n = 0, 1, 2, \ldots$ is the number of electromagnetic energy quanta in the mode, the electromagnetic energy eigenstates are usually denoted $\{|n\rangle\}$, and are called number states or Fock states. The state $|0\rangle$ is the electromagnetic ground state and is often referred to as the vacuum state.

Since the eigenvalues are all non-degenerate, the number states are orthogonal. In addition, since the states are normalized, we have

$$\langle m|n\rangle = \delta_{mn}. \tag{10}$$

The number-state basis is a convenient and complete base to expand various states of the electromagnetic field in. We shall use it several times below.

3 Linear operators

All the dynamics and all measurements of quantum mechanical objects are described by the action of linear operators. Often, but not always, operators are denoted by a hat, e.g., $\hat{A}$. In general, when an operator operates on a state, the ensuing entity is a different state

$$\hat{A}|\psi\rangle = |\psi'\rangle. \tag{11}$$

Note that the order between the operator and the state, and between different operators, is of importance, since operator algebra is non-commutative. Operators operate to the right (left) on kets (bras). Therefore the meaning of the

construction $|\psi\rangle\hat{A}$ is not defined. It suffices to define the action of an operator (and its conjugate) on a ket since the adjoint operator's action on a bra is defined by $\langle\psi|\hat{A}^\dagger \equiv (\hat{A}|\psi\rangle)^\dagger$.

The outer product of two states $|\psi\rangle$ and $|\phi\rangle$ is defined as

$$|\psi\rangle\langle\phi|. \tag{12}$$

Note that this is an operator in contrast to the inner product which is a complex number.

A special operator is the identity operator $\hat{I}$ defined by

$$\hat{I}|\psi\rangle = |\psi\rangle \quad ,\forall \ |\psi\rangle \in \mathcal{H}. \tag{13}$$

The identity operator can be written in a more explicit form. If the set of states $\{|\phi_n\rangle\}$ represent a complete orthonormal basis, then the identity operator can be written

$$\hat{I} \equiv \sum_n |\phi_n\rangle\langle\phi_n|. \tag{14}$$

This expression often comes in handy when doing operator algebra. Furthermore, since the action of any operator is fully described if the operator's action on each of the chosen basis states is known, any operator can be expressed as a sum of outer products. I.e. if

$$\hat{A}|\phi_n\rangle = \sum_m a_{mn}|\phi_m\rangle, \tag{15}$$

then

$$\hat{A} \equiv \sum_{m,n} a_{mn}|\phi_m\rangle\langle\phi_n|. \tag{16}$$

A linear operator satisfies

$$\hat{A}\left(c_1|\psi_1\rangle + c_2|\psi_2\rangle\right) = c_1\hat{A}|\psi_1\rangle + c_2\hat{A}|\psi_2\rangle. \tag{17}$$

In addition

$$\left(\hat{A} + \hat{B}\right)|\psi\rangle = \hat{A}|\psi\rangle + \hat{B}|\psi\rangle. \tag{18}$$

The operator $\hat{A}$:s inverse, $\hat{A}^{-1}$, is defined through

$$\hat{A}\hat{A}^{-1} = \hat{A}^{-1}\hat{A} = \hat{I}. \tag{19}$$

An operator $\hat{U}$ is said to be unitary if its conjugate operator is equal to its inverse, viz.

$$\hat{U}^\dagger = \hat{U}^{-1} \quad \text{or} \quad \hat{U}\hat{U}^\dagger = \hat{U}^\dagger\hat{U} = 1. \tag{20}$$

The commutator bracket of the states $\hat{A}$ and $\hat{B}$ is defined as

$$\left[\hat{A}, \hat{B}\right] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}. \tag{21}$$

If the commutator bracket is zero the operators are said to commute. From the definition it is evident that every operator commutes with itself and the identity operator. From the definition it also follows that

$$\left[\hat{B},\hat{A}\right] = -\left[\hat{A},\hat{B}\right]. \tag{22}$$

If the operators $\hat{A}$ and $\hat{B}$ do not commute then

$$\hat{A}\hat{B}|\psi\rangle \neq \hat{B}\hat{A}|\psi\rangle, \tag{23}$$

in general. (Even if $\hat{A}$ and $\hat{B}$ do not commute it may be possible to find specific states for which the commutator is zero.) The non-commutative algebra is what makes quantum mechanics richer in phenomena than classical physics, but often more difficult to compute. In addition, observable operators that do not commute lead to the concept of complementarity and uncertainty (or indeterminacy) in quantum mechanics.

The eigenstate $|E_n\rangle$ and eigenvalue λ_n of an operator $\hat{A}$ satisfies

$$\hat{A}|E_n\rangle = \lambda_n|E_n\rangle, \tag{24}$$

where the eigenvalues λ_n are complex, in general.

However, all observable or measurable entities correspond to observables, $\hat{O}$, which are Hermitian operators. The definition of a Hermitian operator is

$$\hat{O}^\dagger = \hat{O}. \tag{25}$$

This relation imply that Hermitian operators' eigenvalues are real. In addition eigenstates to $\hat{O}$ with different eigenvalues are orthogonal. If all eigenvalues are different, then the set of (normalized) eigenstates $\{|E_n\rangle\}$ defines a complete orthonormal basis. We have already asserted that the number states, which are eigenstates to the Hermitian energy operator $h\nu(\hat{n}+1/2)$, forms a complete orthonormal set of state vectors.

When one makes a measurement of the observable corresponding to the Hermitian operator $\hat{O}$, the measurement will yield one of the operator eigenvalues as the meter readout. The probability of getting the specific readout λ_n when measuring the state $|\psi\rangle$ is given by

$$P_n = |\langle E_n|\psi\rangle|^2. \tag{26}$$

Hence, a priori the measurement result of a well specified state is in general indeterministic. However, if the measurement yields λ_n as result, then the state collapses into the state $|E_n\rangle$. This is called the von Neumann projection postulate. A subsequent measurement of the state made immediately after the first will yield the result λ_n with certainty.

Since the outcome of quantum mechanical measurements in general are indeterministic, quantum mechanics must be described statistically. The expectation

value of an operator, given that the state vector is $|\psi\rangle$, can be expressed

$$\langle \hat{A} \rangle \equiv \langle \psi | \hat{A} | \psi \rangle = \sum_n P_n \lambda_n = \sum_n |\langle E_n | \psi \rangle|^2 \lambda_n = \sum_n |c_n|^2 \lambda_n. \tag{27}$$

where we have used (26) above, and where $c_n \equiv \langle E_n | \psi \rangle$ is the state vector expansion coefficient in the $\{|E_n\rangle\}$ state basis.

Note that in computing an expression of the type $\langle \psi | \hat{A} | \phi \rangle$, one can either operate with $\hat{A}$ to the right on $|\phi\rangle$ and then take the inner product of $\langle \psi |$ and the result, or operate with $\hat{A}$ to the left on $\langle \psi |$ and then take the inner product of this result with $|\phi\rangle$. The computed value (in general, a complex number) will be the same in the both cases, but the computational difficulty may be significantly different. Hence, before starting such a computation, take a look at the expression and then decide on how to tackle it.

An important operator in quantum mechanics is the density operator $\hat{\rho}$. For a pure state (see below) the density operator is simply the outer product of the state vector, $\hat{\rho} \equiv |\psi\rangle\langle\psi|$. The density operator has a "symmetric" form which makes it convenient to use for operator algebra. The expectation value of an operator can be written

$$\langle \hat{A} \rangle = \mathrm{Tr}\left(|\psi\rangle\langle\psi| \hat{A} \right). \tag{28}$$

Tr denotes the trace and is computed by expanding the state $|\psi\rangle$ in *any* complete orthonormal basis and summing the diagonal elements. Viz.

$$\mathrm{Tr}\left(|\psi\rangle\langle\psi| \hat{A} \right) = \sum_n \langle E_n | \psi \rangle \langle \psi | \hat{A} | E_n \rangle = \sum_n |c_n|^2 \lambda_n. \tag{29}$$

Specifically we see that

$$\mathrm{Tr}(\hat{\rho}) = 1. \tag{30}$$

When manipulating expressions involving the Tr operation, it is useful to remember that the trace operation is invariant under cyclic permutation of its arguments

$$\mathrm{Tr}\left(\hat{A}\hat{B}\hat{C} \right) = \mathrm{Tr}\left(\hat{B}\hat{C}\hat{A} \right). \tag{31}$$

4 Matrix representation

When Werner Heisenberg developed his version of the theory of quantum mechanics in the 1920s he used a methodology based on matrix algebra. Matrix algebra is extremely well suited for the purpose as it is linear, associative, distributive, but non-commutative. That is, the products $\bar{A}\bar{B}$ and $\bar{B}\bar{A}$ of two square matrices $\bar{A}$ and $\bar{B}$ are typically not equal.

To translate the Dirac notation into a matrix formalism one first chooses an ordered basis-vector set. The basis vectors need only to be linearly independent, but for all practical purposes one is well advised to choose an orthonormal set of vectors that span the Hilbert space the system "lives" in. The set of number

states is one commonly used set. In this section we shall use this set, for convenience truncated to the ten least excited states $|0\rangle, \ldots, |9\rangle$. We then use a ten-dimensional, complex, column vector to represent any pure state in this Hilbert space. The states $|0\rangle$ and $|8\rangle$ will be written $(1, 0, \ldots, 0)^T$ and $(0, \ldots, 1, 0)^T$, respectively, where T denotes the transpose. The state $(|0\rangle + \exp(i\pi/5)|3\rangle)/\sqrt{2}$ is represented by the vector $(1/\sqrt{2}, 0, 0, \exp(i\pi/5)/\sqrt{2}, 0, \ldots, 0)^T$ etc. The corresponding bra is the conjugated and transposed column vector (i.e., a row vector). The inner and outer products of the bra and ket vectors will result in a complex scalar and a complex, square matrix, respectively.

An operator $\hat{A}$ is represented by a square matrix $\bar{A}$ with matrix coefficients

$$A_{kl} = \langle \phi_k | \hat{A} | \phi_l \rangle, \tag{32}$$

where, e.g., $|\phi_l\rangle$ is the lth basis-vector ket, c.f. Eq. (16). The operation $\hat{A}|\psi\rangle$ is represented by multiplying the column vector representing $|\psi\rangle$ from the left with the $\bar{A}$ matrix. The result will be a new column matrix.

The structure of the operators will carry over to the matrices. E.g., a Hermitian operator will have an associated Hermitian matrix, and a unitary operator's corresponding matrix will be unitary. As there exist many good computer programs computing and manipulating vectors, matrices, and tensors on the market such as Mathematica, MathLab, and Maple, it is often convenient to use such programs for algebraic manipulation of quantum mechanical expressions. In particular the computers are difficult to beat when it comes to numerical evaluation of expressions. Often symbolic calculations are also possible, but typically the obtained expressions become cumbersome and "ugly" as the size of the Hilbert space grows.

5 The annihilation and the creation operator

Using the number-state basis $\{|n\rangle\}$, it is possible to define an annihilation operator $\hat{a}$ by

$$\hat{a}|0\rangle = 0, \tag{33}$$

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle \quad , n = 1, 2, 3, \ldots. \tag{34}$$

Similarly the (conjugate) creation operator $\hat{a}^\dagger$ is defined by

$$\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle \quad , \forall \ n \geq 0. \tag{35}$$

As an example of the relation (16) above one can alternatively define the creation operator in terms of outer products of number states as

$$\hat{a}^\dagger \equiv \sum_{n=0}^{\infty} \sqrt{n+1}|n+1\rangle\langle n|. \tag{36}$$

Obviously the annihilation operator and the creation operator are different and therefore neither operator is Hermitian. These operators do not correspond

to any observables in quantum optics. However, the product operators $\hat{a}^\dagger\hat{a}$ and $\hat{a}\hat{a}^\dagger$ are both Hermitian. Using the definitions above it is trivial to prove that $\hat{a}^\dagger\hat{a}|n\rangle = n|n\rangle$. Therefore the energy operator of a mode must be $\hat{E} = h\nu(\hat{a}^\dagger\hat{a} + 1/2)$. The operator $\hat{n} = \hat{a}^\dagger\hat{a}$ is called the number operator. Sometimes it is convenient to use the creation and/or annihilation operator to express (or generate) a state from e.g. the vacuum. E.g.

$$|n\rangle = \frac{\left(\hat{a}^\dagger\right)^n}{\sqrt{n!}}|0\rangle. \tag{37}$$

Since $\{|n\rangle\}$ is a complete basis set, any arbitrary state $|\psi\rangle$ can be generated from the vacuum as

$$|\psi\rangle = \sum_{n=0}^{\infty} c_n|n\rangle = \sum_{n=0}^{\infty} c_n \frac{\left(\hat{a}^\dagger\right)^n}{\sqrt{n!}}|0\rangle. \tag{38}$$

We note that

$$\left[\hat{a}, \hat{a}^\dagger\right]|n\rangle = \hat{a}\hat{a}^\dagger|n\rangle - \hat{a}^\dagger\hat{a}|n\rangle = (n+1)|n\rangle - n|n\rangle = |n\rangle \quad ,\forall\ n. \tag{39}$$

Since the number states form a complete basis we can simplify the statement above in the (mathematically) simpler form

$$\left[\hat{a}, \hat{a}^\dagger\right] = \hat{I} = 1. \tag{40}$$

Hence, the Hermitian operators $\hat{a}\hat{a}^\dagger$ and $\hat{a}^\dagger\hat{a}$ are trivially related by $\hat{a}\hat{a}^\dagger = \hat{a}^\dagger\hat{a} + 1$. An interpretation of the operators is that $\hat{a}^\dagger\hat{a}$ correspond to a measurement of the photon number (or energy) by an absorptive meter while $\hat{a}\hat{a}^\dagger$ correspond to the same measurement by an emissive meter. The latter meter is sensitive even to the vacuum state (by spontaneous emission) while the former meter is not.

6 The quadrature operators

By combining the annihilation and the creation operators in a linear superposition one finds the two quadrature operators

$$\hat{a}_1 \equiv \frac{1}{2}\left(\hat{a} + \hat{a}^\dagger\right), \tag{41}$$

$$\hat{a}_2 \equiv \frac{1}{2i}\left(\hat{a} - \hat{a}^\dagger\right). \tag{42}$$

The quadrature operators $\hat{a}_1$ and $\hat{a}_2$ are Hermitian and correspond to a measurement of the in-phase or out-of-phase components of the electric field. To make this more clear, let us look at the classical (complex) notation of the electric field. A (narrow-band) electric field with angular frequency ω is denoted $E\exp(-i\omega t)$. However, the real electrical field is given by $\mathrm{Re}\{E\exp(-i\omega t)\} =$

$\mathrm{Re}\{E\}\cos(\omega t) + \mathrm{Im}\{E\}\sin(\omega t)$. Hence, the field is uniquely decomposed in slowly varying quadrature components $\mathrm{Re}\{E\} = (E + E^*)/2$ and $\mathrm{Im}\{E\} = (E - E^*)/(2i)$. The corresponding operators are $\hat{a}_1$ and $\hat{a}_2$, and they correspond to a perfect homodyne measurement. Since an electric field is a continuous observable, the respective eigenvalues of the associated eigenstates have continuous spectra.

Since $\hat{a}_1$ and $\hat{a}_2$ are linearly independent combinations of the $\hat{a}$ and $\hat{a}^\dagger$ operators, all operators formed by combinations of $\hat{a}$ and $\hat{a}^\dagger$ can also be expressed in $\hat{a}_1$ and $\hat{a}_1$. Specifically the Hermitian energy operator $\hat{E}$ can be expressed as $\hat{E} = h\nu(\hat{a}_1^2 + \hat{a}_2^2)$. (Check this!) The quadrature operators do not commute. The commutator is $[\hat{a}_1, \hat{a}_2] = i/2$. This follows from (40).

7 The coherent state

Although the operator $\hat{a}$ is non-Hermitian, it has an (over)-complete set of associated eigenstates. The coherent state is denoted $|\alpha\rangle$, where α is a complex number. The defining equation of a coherent state is

$$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle, \tag{43}$$

where $\alpha \in \mathcal{C}$.

The number state expansion of a coherent state is

$$|\alpha\rangle = e^{-\frac{|\alpha|^2}{2}} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}}|n\rangle. \tag{44}$$

Note that the coherent states with $\alpha = 1, 2, \ldots$, must be labeled in such a way as to distinguish them from the number states $|1\rangle, |2\rangle, \ldots$. However, it is clear from (44) that $\alpha = 0$ represents the electromagnetic ground state, the vacuum state.

The probability of detecting n photons in a coherent state $|\alpha\rangle$ is given by (44) as

$$P_n = |\langle n|\alpha\rangle|^2 = \left| e^{-\frac{|\alpha|^2}{2}} \frac{\alpha^n}{\sqrt{n!}} \right|^2 = e^{-|\alpha|^2} \frac{|\alpha|^{2n}}{n!}. \tag{45}$$

Hence, the photon-count statistics is Poissonian. One finds that the expectation value and the variance of the photon number to be

$$\langle \hat{n} \rangle = \langle (\Delta \hat{n})^2 \rangle = |\alpha|^2, \tag{46}$$

where $\Delta\hat{n}$ is defined by $\Delta\hat{n} \equiv \hat{n} - \langle \hat{n} \rangle$. The light from a good, ordinary laser is approximately in a coherent state for measurement times shorter than the coherence time of the laser.

The expectation value for the operators $\hat{a}_1$ and $\hat{a}_2$ are

$$\langle \hat{a}_1 \rangle = \mathrm{Re}\{\alpha\} \quad \text{and} \quad \langle \hat{a}_2 \rangle = \mathrm{Im}\{\alpha\} \tag{47}$$

and

$$\langle \Delta \hat{a}_1^2 \rangle = \langle \Delta \hat{a}_2^2 \rangle = \frac{1}{4} \tag{48}$$

for a coherent state $|\alpha\rangle$. Check this using the commutator bracket and the fact that if $\hat{a}|\alpha\rangle = \alpha|\alpha\rangle$ then $\langle\alpha|\hat{a}^\dagger = \langle\alpha|\alpha^*$.

8 Modes and states, multi-mode states

It is important to distinguish between modes and states. The modes describe the vibration-, rotation-modes, etc., of some system while the state vector describes the excitation of these modes. For electromagnetic fields the modes are given by the solutions of Maxwell's equations (and the associated boundary conditions) while the states are given by the solutions of Schrödinger's equation (and the associated initial conditions). Every mode has an associated Hilbert space and unique associated operators. So far we have dealt with single mode states. To describe a multi-mode state of e.g. one electromagnetic mode in the vacuum state $|0\rangle$, and one two level atom in the excited state $|e\rangle$, we write

$$|0\rangle \otimes |e\rangle = |0, e\rangle, \tag{49}$$

where $\otimes$ denotes the tensor product and the right-most term denotes a simplified notation of the tensor product of the states. When writing the associated bra to this state, the notational order of the modes is usually not altered. Hence $|0, e\rangle^\dagger = \langle 0, e|$. Suppose that the electromagnetic mode has some associated operator $\hat{E}$ and that the atom has an associated operator $\hat{A}$. Since $\hat{E}$ and $\hat{A}$ operate on different Hilbert spaces they commute. Furthermore

$$\hat{E}\hat{A}|0\rangle \otimes |e\rangle = (\hat{E}|0\rangle) \otimes (\hat{A}|e\rangle). \tag{50}$$

If the modes are similar, e.g. two spatially different but otherwise similar electromagnetic modes, they formally have the same set of associated operators. In this case it is in general necessary to index the operators to show which operator operates on which mode.

9 Entangled states

A fundamental notion in quantum mechanics is a linear superposition. We already encountered superposition states in (1) above. However, the combination of multi-mode states and superposition states leads to the consequence that quantum mechanics is a non-local theory. This consequence of the superposition principle in quantum mechanics has troubled and/or intrigued physicists almost since the invention (or discovery?) of quantum mechanics.

Assume that we have two electromagnetic modes in a superposition of a zero-photon state (a vacuum state) and a one photon state. One way of writing such a state is:

$$(|0\rangle + |1\rangle)/\sqrt{2} \otimes (|0\rangle + |1\rangle)/\sqrt{2} = \frac{1}{2}\left(|0,0\rangle + |1,0\rangle + |0,1\rangle + |1,1\rangle\right). \tag{51}$$

We note that the joint state is the tensor product of two single-mode states. Hence, according to the von Neumann projection postulate, if we measure the photon number of the first mode, the probability of measuring zero photons is $1/2$, and in this case the post-measurement state becomes $|0\rangle \otimes (|0\rangle + |1\rangle)/\sqrt{2}$. In the remaining half cases we will measure the photon number of the first mode to be unity and the state will collapse to the state $|1\rangle \otimes (|0\rangle + |1\rangle)/\sqrt{2}$. We note that the state of the second mode is unaffected by the measurement outcome of the first.

A different possibility of making a superposition state where both modes are in a superposition of zero and one photons is the state

$$(|1,0\rangle + |0,1\rangle)/\sqrt{2}. \tag{52}$$

We note that this state is impossible to factor into a product state of the two modes. Such a state is called an entangled state. If we measure the photon number of the first mode, in half the cases we will measure zero photons. In this case the joint state will collapse into the state $|0,1\rangle$. If, on the other hand we measure the first mode to contain one photon, the state collapses into the state $|1,0\rangle$. Hence, *the post-measurement state of the second mode is contingent on the measurement result of the first mode.* According to the von Neumann postulate this reduction of the state is instantaneous. Hence, even if the two modes are separated by large distances the state of the second mode instantaneously reacts to the "collapse" of the state of the first mode. Quantum mechanics is therefore said to be a non-local theory. In addition, since the post measurement states $|0,1\rangle$ and $|1,0\rangle$ are orthogonal, the joint state (52) is said to be maximally entangled.

Entanglement forms the core of the new discipline quantum information. By synthesis, it has been shown that entanglement can be harnessed to solve certain tasks, such as quantum teleportation, quantum cryptography and quantum computation, that are impossible using classical object. Conversely, in, e.g., a quantum computer it is inevitable to create entangled states because all quantum computing algorithms uses conditional superpositions (in, e.g., so-called CNOT gates) to achieve their efficiency relative to classical computers. Hence, the generation, manipulation and classification of entangled states has been central in quantum optics for the past twenty years.

10 Pure and mixed states

In general there is always (wanted or unwanted) interaction between modes. Quite often one is faced with the experimental reality that one cannot control or measure a large number of these modes. Since, as we saw in the last section, quantum mechanics is non-local, that is, the state of some mode is contingent of the state of one or many other modes, one seems stuck in a impasse. In this case the way out is to write down the density operator of total system and to trace out the unwanted or neglected states. This will give a correct description of

the outcome of any subsequent local measurement or operation in the ensemble averaged sense. Suppose that we are interested in the second mode in (51). In this case the reduced density operator of the system becomes

$$\mathrm{Tr}_1(\hat{\rho}) = \sum_n \langle n_1|\hat{\rho}|n_1\rangle = (|0\rangle\langle 0| + |1\rangle\langle 0| + |0\rangle\langle 1| + |1\rangle\langle 1|)/2, \tag{53}$$

where the index 1 denotes that the we make only a partial trace (over the first mode). We note that the ensuing density operator can be written as the outer product of a ket and its associated bra, $\hat{\rho} = (|0\rangle + |1\rangle)(\langle 0| + \langle 1|)/2$. Therefore the state is said to be pure. This is a consequence of the fact that the joint two-mode state was not entangled. The density operator of all pure states satisfies $\mathrm{Tr}\left(\hat{\rho}^2\right) = 1$. It is easy to confirm that (53) satisfies this relation.

If we trace out the first mode of the state (52) a different situation arises.

$$\begin{aligned} \mathrm{Tr}_1(\hat{\rho}) &= \textstyle\sum_n \langle n_1|\frac{1}{2}\left(|1,0\rangle\langle 1,0| + |1,0\rangle\langle 0,1| + |0,1\rangle\langle 1,0| + |0,1\rangle\langle 0,1|\right)|n_1\rangle \\ &= \tfrac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|) \end{aligned} \tag{54}$$

This state cannot be written as an outer product of a ket and its associated bra and it is called a mixed state. One interpretation is that in principle one could have known the state of the second mode state upon a measurement of the first mode. If we ignore this information, the state is described by a proper statistical mixture of the $|0\rangle$ and $|1\rangle$ state. It is easy to confirm that for this state $\mathrm{Tr}(\hat{\rho}) = 1$ (this is true for all states, mixed or pure) but that $\mathrm{Tr}\left(\hat{\rho}^2\right) = 1/2 < 1$. The last inequality is a signature of a mixed state.

It is important to appreciate the difference between a mixed and a pure state. The former is more akin to our everyday experiences. We may have limited knowledge about certain results, e.g., whether or not we have a winning lottery ticket or not. A good way to quantify our information is to assign a probability to the possible outcomes. This probability is of course contingent on our prior knowledge, e.g., how many lottery tickets are sold. We all understand that the situation both before and after the lottery drawing is an "either win or lose" situation. That is, the possible "system states" are mutually exclusive even before the actual drawing, when the actual system state is revieled is made.

A superposition is rather different. In a superposition both possibilities co-exist until a measurement is made. We have little everyday experience of this situation, e.g., that a photon, which is indivisible, must be assigned a probability amplitude of each of two or several possibilities that, if they are measured, result in mutually exclusive outcomes.

A photon passing a double slit is a good example of a statistical mixture vs. a superposition. Assume that one illuminates an area much larger than the slit widths. The most likely outcome is then that the photon is reflected or absorbed by the membrane the two slits are carved into. The situation pass or not pass is described by a mixture of the two possibilities where, based on the geometry of the illuminated spot and the double slit we can assign a probability

of transmission and a probability of non-transmission. There are several reasons why this situation is best describes by a statistical mixture of states. The first is ignorance. We typically don't care about the situation when the photon don't pass the slits, and therefore we will not worry about a reflected or absorbed photon's further history. It is then convenient to simply assign an *a priori* probability to the two cases (that are mutually exclusive and also complete so that the two probabilities sum to unity).

However, if the photon is absorbed by the membrane there is a deeper reason to assign an *a priori* probability to the no-pass event. The reason is that in principle Nature makes a "measurement" of whether the photon passes or not. Thus, in principle this information is available to us (e.g., in the form of a minuscule heating of the membrane). In practice we probably don't care about this information, and even if we did, our lack of preparation and control of the membrane may make it impossible to obtain this information in practice, although it is there in principle. If, by any means (if even only in principle) information about one outcome rather than the other is available, the possibilities must be described by a mixed state.

In contrast, which path the photon took through the slits should be described by a superposition. The reason is that the slits are (or should be) prepared in such a way that it is impossible, even in principle, to know which path the photon took. Here, the physical implementation of the slits does matter. If the slit walls are too soft, or the membrane too light, the recoil of the photon being diffracted through one slit or another may leave a "fingerprint" allowing us to deduce (perhaps only in principle) which slit the photon passed through. If so, also this situation should be described by a mixed state and not by a superposition. This would also mean that no interference will be present after the slits. In a typical Young's experiment, however, the slits are too rigid and the membrane much too heavy to experience a sufficient recoil to "measure" which slit the photon took. Thus it is impossible, even in principle, to deduce the path information. As a result interference between the two path possibilities will appear after the slits.

In short, indistinguishability leads to superpositions, interference and coherence. Distinguishability (if even only in principle) prohibits the named three. The latter situation is formally handled by mixed density matrices in quantum theory, reflecting the fact that in principle information about some event or path is available but that this information is ignored or inaccessible in practice.

11 Temporal evolution

We have seen above that a state may change as a consequence of measurement. However, even if the state is left by itself it will evolve dynamically. The evolution will be unitary, i.e., a rotation of the state vector in Hilbert space. A unitary operator is defined by (20) above. As a consequence the norm of the state vector will always be preserved under a unitary transformation, viz. if the

normalized state $|\psi\rangle$ evolves unitarily to the state $|\phi\rangle = \hat{U}|\psi\rangle$ then

$$\langle\phi|\phi\rangle = \langle\psi|\hat{U}^\dagger\hat{U}|\psi\rangle = \langle\psi|\hat{I}|\psi\rangle = \langle\psi|\psi\rangle = 1. \tag{55}$$

In addition unitary rotation of any orthonormal set of states will leave the set orthonormal. If $|\psi_m\rangle$ and $|\psi_n\rangle$ are two arbitrary state vectors in the set so that $\langle\psi_m|\psi_n\rangle = 0$, then the new states $|\phi_m\rangle = \hat{U}|\psi_m\rangle$ and $|\phi_n\rangle = \hat{U}|\psi_n\rangle$ satisfy

$$\langle\phi_m|\phi_n\rangle = \langle\psi_m|\hat{U}^\dagger\hat{U}|\psi_n\rangle = \langle\psi_m|\hat{I}|\psi_n\rangle = \langle\psi_m|\psi_n\rangle = 0. \tag{56}$$

There are two principal ways of treating the temporal evolution of a quantum system. In the first, one assumes that all operators are independent of time and assigns the temporal dynamics to the state. This is called the Schrödinger picture. In the second, one lets the states be time independent and assign the temporal evolution to the operators. This is the Heisenberg picture.

11.1 The Schrödinger picture

The Schrödinger equation in the Dirac notation is

$$i\hbar\frac{d}{dt}|\psi\,(t)\rangle = \hat{H}|\psi\,(t)\rangle, \tag{57}$$

where we have assumed that the Hamiltonian $\hat{H}$ has no explicit time dependence. We can formally integrate (57) to obtain

$$|\psi(t)\rangle = \exp(-i\hat{H}t/\hbar)|\psi(0)\rangle = \hat{U}(t)|\psi(0)\rangle. \tag{58}$$

In this equation (and other equations involving functions of an operator) the function of an operator is defined in terms of its Taylor expansion. E.g.,

$$\exp(-i\hat{H}t/\hbar) \equiv 1 + \frac{-i\hat{H}t}{1!\hbar} + \frac{(-i\hat{H}t)^2}{2!\hbar^2} + \ldots \quad . \tag{59}$$

Since $\hat{H}$ is an Hermitian operator (and therefore has real eigenvalues) one can easily prove that the operator $\exp(-i\hat{H}t/\hbar)$ is unitary. Hence, the temporal evolution of a state in the Schrödinger picture is governed by a unitary operator $\hat{U}(t) = \exp(-i\hat{H}t/\hbar)$.

If the initial state is mixed it is convenient to use the density operator to describe the state. The corresponding equation of motion for the density operator is

$$\hat{\rho}(t) = \hat{U}\hat{\rho}(0)\hat{U}^\dagger, \tag{60}$$

and it fulfills

$$i\hbar\frac{d\hat{\rho}\,(t)}{dt} = \left[\hat{H}, \hat{\rho}\,(t)\right]. \tag{61}$$

Note that the density operator is particular in this respect. Although it is formally an operator, it is time dependent in the Schrödinger picture.

11.2 The Heisenberg picture

An alternative way of treating the temporal evolution of quantum mechanical systems is to make the operators time dependent and the states time independent. This will make all expectation values (which are the measurable entities in the theory) time dependent, although the states are time independent. Starting from the temporal evolution of $\hat{\rho}$ in the Schrödinger picture (61) the expectation value of an arbitrary operator, $\hat{A}$, for a state with the density operator $\hat{\rho}$ is given by

$$\begin{aligned} \langle \hat{A} \rangle (t) &= \mathrm{Tr}\left(\hat{\rho}(t)\hat{A}\right) = \mathrm{Tr}\left(\hat{U}(t)\hat{\rho}(0)\hat{U}^{\dagger}(t)\hat{A}\right) \\ &= \mathrm{Tr}\left(\hat{\rho}(0)\hat{U}^{\dagger}(t)\hat{A}\hat{U}(t)\right) = \mathrm{Tr}\left(\hat{\rho}_H \hat{A}_H(t)\right), \end{aligned} \tag{62}$$

where the time-dependent operator $\hat{A}$ and the density operator in the Heisenberg picture are defined by

$$\hat{A}_H(t) = \hat{U}^{\dagger}(t)\hat{A}\hat{U}(t), \tag{63}$$

$$\hat{\rho}_H = \hat{U}^{\dagger}(t)\hat{\rho}(t)\hat{U}(t) = \hat{\rho}(0). \tag{64}$$

Hence, in the Heisenberg picture the density operator is time independent. So is the Hamiltonian since

$$\hat{H}_H(t) = \hat{U}^{\dagger}(t)\hat{H}\hat{U}(t) = \hat{U}^{\dagger}(t)\hat{U}(t)\hat{H} = \hat{H}, \tag{65}$$

where we used (58) and the fact that $\hat{H}$ commutes with itself (as any operator does).

The Schrödinger equation in the Heisenberg picture (called the Heisenberg equation of motion) can be written

$$i\hbar \frac{d\hat{A}_H(t)}{dt} = \left[\hat{A}_H(t), \hat{H}\right]. \tag{66}$$

This equation should not be confused with (61), which pertains to the density operator, the only operator which evolves in time in the Schrödinger picture.

The Schrödinger and the Heisenberg pictures are equivalent and mutually consistent. Which picture to use in any specific problem is a matter of convenience and personal taste. Occasionally it is convenient to solve a problem in the Heisenberg picture, express the initial state in terms of operations on the vacuum state (like in equation (37)) and then operate with the time-dependent operator(s). The ensuing time-dependent state-vector will be the the Schrödinger picture solution.

12 The phase shifter

A phase shift is really not anything but a time displacement. Therefore, not surprisingly, the phase-shift Hamiltonian is the free Hamiltonian of the mode.

If the mode is a harmonic oscillator of the electromagnetic field, the phase-shift Hamiltonian is given by

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

where $\omega = 2\pi\nu$, and ν is the (optical) frequency. Often the zero point energy $1/2$ is suppressed in the equation since it gives a fixed phase shift to every state and therefore trivially can be removed.

The phase shifter's unitary time-evolution operator is then given by (58)

$$\hat{U}(t) = e^{-i\frac{\hat{H}}{\hbar}t} = e^{-i\omega t\hat{n}}. \tag{68}$$

The number states therefore evolve like

$$|\psi_n(t)\rangle = e^{-i\omega t\hat{n}}|n\rangle = e^{-i\omega tn}|n\rangle, \tag{69}$$

but, as we stated above, states differing only in an overall phase-factor are equivalent. Therefore the number states remain invariant under phase shifting. However, a general state $|\psi(0)\rangle = \sum_{n=0}^{\infty} c_n|n\rangle$ is affected by a phase shifter and its temporal evolution becomes

$$|\psi(t)\rangle = \sum_{n=0}^{\infty} c_n e^{-i\omega tn}|n\rangle. \tag{70}$$

If the state $|\psi(t)\rangle$ is a coherent state (70) can be simplified. In this case $e^{-i\omega t\hat{n}}|\alpha\rangle = |e^{-i\omega t}\alpha\rangle$.

13 The beam splitter

In this last section of the PM we will apply the Dirac formalism to a simple but non-trivial optical component, the beam splitter. It is important to remember that throughout the PM we have outlined non-relativistic quantum mechanics. In the lab, we usually deal with propagating pulses of light, but in the formalism these pulses are modeled by stationary quantized modes (particle in a box). Hence, *the spatial evolution of a temporal mode is modeled by the temporal evolution of a spatial mode.* It is important to keep this in mind when thinking about models for various quantum systems.

In the case of a beam splitter, in reality we have a component combining two propagating modes into two other propagating modes in a fs time scale. We usually model this system by considering two modes in two separate resonators interacting for a fixed (and compared to the field's oscillation cycle, usually a fairly long) time. We then make predictions about the joint state after the interaction is over. It is then obvious that the interaction time and the interaction strength of the two resonator modes both must influence the final state of the system. A real beam splitter, on the other hand, is usually characterized by

a single number, e.g., its reflectivity. We shall see that this single number is not sufficient to characterize a beam splitter, but that since absolute reflection and transmission phase-shifts often are unimportant in applications, this single number usually suffices for users.

The beam splitter a linear device coupling two modes to each other. The Hamiltonian, in the rotating wave approximation can be written

$$\hat{H} = \hbar\theta\left(\hat{a}^\dagger\hat{b} + \hat{a}\hat{b}^\dagger\right), \tag{71}$$

where $\hat{a}$ and $\hat{b}$ are the annihilation operators for the a- and b-mode, and θ is a parameter characterizing the oscillator interaction strength. The Heisenberg equation of motion (66) becomes

$$\begin{aligned}\frac{d\hat{a}_H(t)}{dt} &= \frac{i}{\hbar}\left[\hat{H}, \hat{a}_H(t)\right] = i\theta\left[\hat{a}_H^\dagger(t)\hat{b}_H(t) + \hat{a}_H(t)\hat{b}_H^\dagger(t), \hat{a}_H(t)\right] \\ &= i\theta\left\{\left(\hat{a}_H^\dagger(t)\hat{a}_H(t) - \hat{a}_H(t)\hat{a}_H^\dagger(t)\right)\hat{b}_H(t)\right. \\ &\quad \left. + \left(\hat{a}_H(t)\hat{a}_H(t) - \hat{a}_H(t)\hat{a}_H(t)\right)\hat{b}_H^\dagger(t)\right\} = -i\theta\hat{b}_H(t). \end{aligned} \tag{72}$$

In the same manner the equation for the $\hat{b}$ operator becomes

$$\frac{d\hat{b}_H(t)}{dt} = -i\theta\hat{a}_H(t). \tag{73}$$

The coupled, linear equation-system has the solution

$$\hat{a}_H(t) = \hat{a}\cos\theta t - i\hat{b}\sin\theta t, \tag{74}$$

$$\hat{b}_H(t) = \hat{b}\cos\theta t - i\hat{a}\sin\theta t. \tag{75}$$

It is convenient to express this as a matrix

$$\begin{pmatrix} \cos\theta t & -i\sin\theta t \\ -i\sin\theta t & \cos\theta t \end{pmatrix}. \tag{76}$$

We see that the annihilation operators periodically evolve into each other with the period $\theta t = \pi/2$ and they "revive" in a period $\theta t = \pi$. This "revival" may seem strange, but this is a characteristic of any two linearly coupled harmonic oscillators.

The "half-silvered mirror" which often is discussed in physics textbooks, is a beam splitter with a 50 % transmission. We see that quantum mechanically such a beam splitter is realized if the interaction strength is chosen according to $\theta t = \frac{\pi}{4} + k\frac{\pi}{2}$, where k is an integer.

In the general case we can independently add phase shifts to both the beam

splitter input ports. This will add independent phase shifts to the $\hat{a}$ and $\hat{b}$ modes. The general beam splitter matrix can therefore be expressed

$$\begin{pmatrix} \exp(i\Phi_a)\cos\theta t & \exp(i\Phi_b)\sin\theta t \\ -\exp(-i\Phi_b)\sin\theta t & \exp(-i\Phi_a)\cos\theta t \end{pmatrix}. \tag{77}$$

It is easy to check that the matrix above is unitary.

13.1 Splitting states in a 50/50 beam splitter

As stated above, the 50/50 beam splitter (which is generic to most interference experiments) requires $\theta t = \frac{\pi}{4}$. With this choice the corresponding unitary operator becomes

$$e^{-i\frac{\pi}{4}\left(\hat{a}^\dagger\hat{b}+\hat{a}\hat{b}^\dagger\right)}|\psi_a,\psi_b\rangle. \tag{78}$$

However, for simple states it is actually easiest to initially work in the Heisenberg picture. For this end we use (74) and (75). The prescription then tells us to make the substitutions

$$\hat{a}^\dagger \to \frac{1}{\sqrt{2}}\left(\hat{a}^\dagger + i\hat{b}^\dagger\right), \tag{79}$$

$$\hat{b}^\dagger \to \frac{1}{\sqrt{2}}\left(\hat{b}^\dagger + i\hat{a}^\dagger\right), \tag{80}$$

to get the states after the beam splitter.

13.2 Input state: $|1\rangle \otimes |0\rangle$

Let us start by examining what happens when a single photon is incident on a 50/50 beam splitter. A single photon is in the a-mode and nothing (the vacuum) is the initial state of the b-mode. The respective states can be written $|1\rangle = \hat{a}^\dagger|0\rangle$ and $|0\rangle$. Substitution of the initial to final operators give

$$|1,0\rangle = \hat{a}^\dagger|0,0\rangle \to \frac{1}{\sqrt{2}}\left(\hat{a}^\dagger + i\hat{b}^\dagger\right)|0,0\rangle = \frac{1}{\sqrt{2}}\left(|1,0\rangle + i|0,1\rangle\right). \tag{81}$$

We see that the probability of detecting one-photon in the a-mode after the beam splitter is 50 %, and that every time we measure one photon in the a-mode, no photon will be detected in the b-mode. If, on the other hand, no photon is detected in the a-mode, then exactly one photon will be detected in the b-mode. Hence, energy is always preserved. In the ensemble-average meaning the beam splitter transmission is 50 %. However, in every single realization of the experiment the transmittivity is either unity or zero (with equal probability). This is a manifestation of the quantization of energy in combination with the initial condition.

13.3 Input state: $|1\rangle \otimes |1\rangle$

If both the impinging modes are in a single photon eigenstate we get

$$\begin{aligned} |1,1\rangle &= \hat{a}^\dagger \hat{b}^\dagger |0,0\rangle \rightarrow \frac{1}{\sqrt{2}}\left(\hat{a}^\dagger + i\hat{b}^\dagger\right)\frac{1}{\sqrt{2}}\left(\hat{b}^\dagger + i\hat{a}^\dagger\right)|0,0\rangle \\ &= \frac{1}{2}\left(i\left(\hat{a}^\dagger\right)^2 + i\left(\hat{b}^\dagger\right)^2\right)|0,0\rangle \\ &= \frac{i}{\sqrt{2}}\left(|2,0\rangle + |0,2\rangle\right) = \frac{1}{\sqrt{2}}\left(|2,0\rangle + |0,2\rangle\right). \end{aligned} \tag{82}$$

Let us compare this case with the case when the impinging particles are classical. In this latter case every particle has a 50 % chance of transmission, yielding the "classical" density operator

$$\hat{\rho}_{class.} = \frac{1}{4}|2,0\rangle\langle 2,0| + \frac{1}{2}|1,1\rangle\langle 1,1| + \frac{1}{4}|0,2\rangle\langle 0,2|. \tag{83}$$

We see that the probabilities of measuring one particle in each output becomes $1/2$ and the probability of detecting two particles in the a- and b-output is $1/4$, respectively. Inspection of (82) shows that photons are non-classical in that they will always exit the beam splitter both in the same output. The two photons will never go separate ways. This is a quantum mechanical interference effect (in quantum mechanics probability amplitudes, which may be negative, are added, not probabilities which are always positive). This is the first example which shows the rich, and sometimes non-intuitive, dynamics of even simple quantum systems.