1 Some useful algebraic structures.

1.1 Groups.

A *group* is a set of elements G together with an operation $\bullet$ that combines any two elements and gives another element of the group.

- Closure: $\forall\ a, b \in G$, $a \bullet b \in G$.
- Associativity: $\forall\ a, b, c \in G$, $(a \bullet b) \bullet c = a \bullet (b \bullet c)$.
- Existence of the identity element: $\exists\ e \in G$ such that, $\forall\ a \in G$, $a \bullet e = e \bullet a = a$
- Existence of the inverse: $\forall\ a \in G$, $\exists\ b \in G$ such that $a \bullet b = b \bullet a = e$.

The concept of group is particularly important in physics because the set of symmetries of a physical system is a group. In this case the product of two elements consists just in performing the two symmetry operation in sequence: the result is a possibly new operation that leaves the system invariant.

1.1.1 Examples and exercises.

- The set of integer numbers $\mathbf{Z}$ (that is $\ldots, -2, -1, 0, 1, 2, \ldots$), together with the standard addition form a group $(\mathbf{Z}, +)$

This group enjoys an additional property, that is the operation is commutative: $\forall\ a, b \in \mathbf{Z}$ we have $a + b = b + a$. This type of groups is called Abelian.

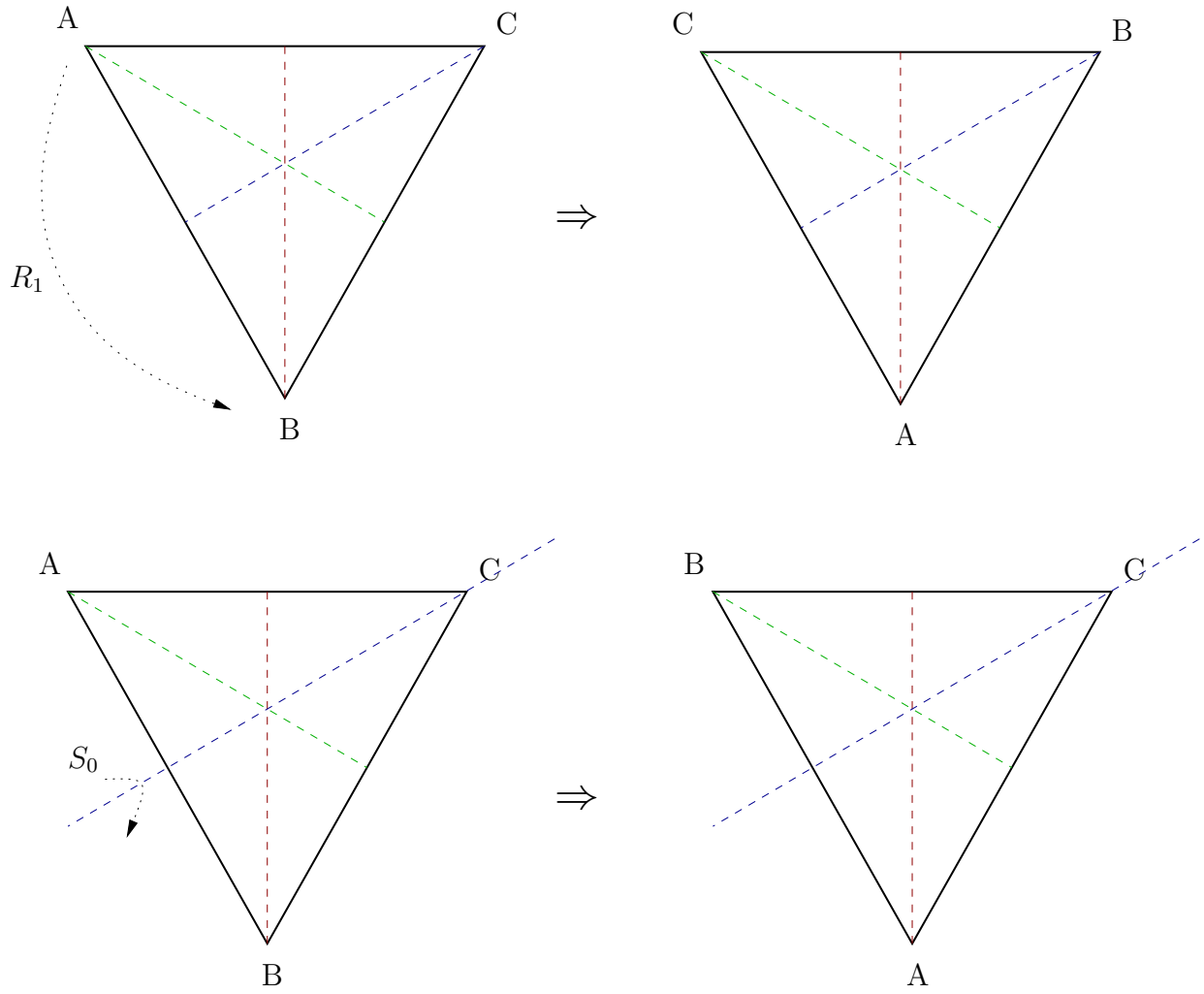
- Consider an equilateral triangle: a rotation by 120 degrees ($2\pi/3$ radians) around the center of the triangle leaves the object invariant.

Notice that these operations are *not* the only symmetries of the triangle! We can perform also reflection along the three altitudes and leave the triangle unchanged. The group generated by all symmetries is called D_3 (it's one of the Dihedral groups). This group contains a finite number of elements and is not Abelian (non-Abelian). See exercise below.

- Consider a sphere: any rotation around an axis passing through the origin of the sphere leaves the sphere unchanged. The set of all these rotations forms a group that we will analyze in some detail in this course.

This group contains an infinite numbers of elements, since the angle of the rotation is a continuous parameter. As we will see this group is non-Abelian.

Exercise: Consider the group D_3. This group is generated by the following two operations:



1. Compose these two symmetries in all possible ways and write down all elements of D_3. How many elements are contained in D_3 ?

2. Write down all possible products between two elements in D_3 and prove that the group is non-Abelian.

1.2 Vector spaces.

A vector space is a set of elements that can be summed and rescaled: it represents an abstraction of the usual Euclidean space. To be precise, a *real vector space* V is an Abelian group with respects to the addition; moreover each element of $v \in V$ can be multiplied

(rescaled) by a real number a and $av \in V$. This scalar multiplication must have the following properties:

- Distributivity with respect to the vector addition: $\forall\ a \in \mathbf{R}$ and $\forall\ v,\ w \in V$ we have $a(v+w) = av + aw$;
- Distributivity with respect to the real number addition: $\forall\ a,\ b \in \mathbf{R}$ and $\forall\ v \in V$ we have $(a+b)v = av + bv$;
- $\forall\ a,\ b \in \mathbf{R}$ and $\forall\ v \in V$ we have $a(bv) = (ab)v$;
- Multiplication by the identity and zero: $\forall\ v \in V$ we have $1v = v$ and $0v = 0$.

A *complex vector space* is defined in a similar way just by allowing rescaling of the vectors with complex, instead of real numbers. Then in the axioms above a, b will belong to $\mathbf{C}$.

Vector spaces play a central role in physics. In classical mechanics the position of a point-particle is specified by a vector in the Euclidean space. In Quantum mechanics the state of a system is specified by the wavefunction which, as we will see, is an element in a complex vector space.

Let me now recall the concept of linearly independent vectors

- A set of vectors $\{v_1, v_2, \ldots, v_m\}$ is *linearly independent* if $a_1 v_1 + \ldots + a_m v_m = 0$ (with $a_i \in \mathbf{R}$ for real vector spaces, while $a_i \in \mathbf{C}$ for complex spaces) implies that $a_1 = \ldots = a_m = 0$.
- If it exists a maximum number of linearly independent vectors n, then n is the dimension of the vector space. A set of n linearly independent vectors is called *basis*.

This implies that a vector space V of dimension n can be "represented"[1] as the Euclidean space ($\mathbf{R}^n$ for real vector spaces and $\mathbf{C}^n$ for complex ones). Consider a basis $\{v_1, v_2, \ldots, v_n\}$ for this space; then we have the following

Theorem: each vector $v \in V$ has a *unique* decomposition in terms of $\{v_1, v_2, \ldots, v_n\}$

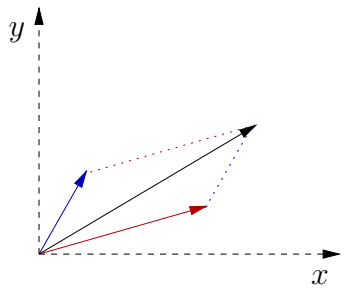
$$v = a_1 v_1 + \ldots + a_n v_n\ . \tag{1.1}$$

Proof "by contradiction". Suppose that there are two different such decompositions: $v = \sum_{i=1}^n a_i v_i$ and $v = \sum_{i=1}^n b_i v_i$ with $a_i \neq b_i$ at least for one value of i. Then we can take the difference between these two decompositions and get: $0 = \sum_{i=1}^n (a_i - b_i) v_i$. This contradicts the hypothesis that $\{v_1, v_2, \ldots, v_n\}$ forms a basis. The n numbers a_i are called *coordinates* of v in the basis $\{v_1, v_2, \ldots, v_n\}$.

[1] We will see next week what this means exactly.

1.2.1 Examples and exercises.

- The 2-dimensional Euclidean space is the standard example of a vector space.



The 2-dimensional Euclidean space: the elements of this real vector space are arrows on a plane whose length can be rescaled and that can be summed in the usual way.

Exercises:

1) Consider the set of polynomial with real coefficients of degree 2: $3x+4$ and $x^2+\sqrt{2}$ are examples of such polynomials and $\sum_{i=0}^{2} a_i x^i \equiv a_2 x^2 + a_1 x + a_0$ with $a_i \in \mathbf{R}$ is the most general element.

- Show that this set forms a vector space with the standard addition between polynomial and with the scalar multiplication with any real number b defined as: $b(\sum_{i=0}^{2} a_i x^i) = \sum_{i=0}^{2} (b a_i) x^i$.
- What is the dimension of this vector space ?

2) Consider the following pairs of vectors in $\mathbf{C}^3$:

$$a) \qquad v = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} \quad , \quad w = \begin{pmatrix} 4 \\ 5 \\ 6 \end{pmatrix} \quad ; \tag{1.2}$$

$$b) \qquad v = \begin{pmatrix} 1 \\ 1 \\ 2 \end{pmatrix} \quad , \quad w = \begin{pmatrix} 2 \\ 2 \\ 4 \end{pmatrix} \quad ; \tag{1.3}$$

$$c) \qquad v = \begin{pmatrix} 1 \\ i \\ -i \end{pmatrix} \quad , \quad w = \begin{pmatrix} i \\ -1 \\ 1 \end{pmatrix} \quad . \tag{1.4}$$

Check whether these pairs of vectors linearly are linearly independent.

1.3 Scalar products and Hilbert Spaces.

We are interested in vector spaces that have an additional structure: a **scalar product** (sometimes I will use the equivalent denomination "inner product"). The inner product

is a bilinear map from $V \times V \to \mathbf{R}$ ($V \times V \to \mathbf{C}$ for complex vector spaces). Let me focus on the complex case:

- linearity: $\forall\ a_i \in \mathbf{C}$ and $\forall\ w, v_i \in V$ we have $(w, a_1 v_1 + a_2 v_2) = a_1 (w, v_1) + a_2 (w, v_2)$ and $(a_1 v_1 + a_2 v_2, w) = \bar{a}_1 (v_1, w) + \bar{a}_2 (v_2, w)$
- conjugation symmetry: $\forall\ w, v \in V$ we have $(w, v) = \overline{(v, w)}$.

Notice that this last property implies that $(v, v) \in \mathbf{R}\ \forall\ v \in V$. Then it makes sense to require that

- $\forall\ v \neq 0$ in V we have $(v, v) > 0$

When this additional property is satisfied the scalar product is said to be *positive definite*. The scalar product of a vector with itself is called *norm*: $||v||^2 \equiv (v, v)$. In our applications to Quantum Mechanics we will be focusing on positive definite scalar products. On the contrary, for instance in special relativity one deals with a vector space with a non-positive definite scalar product.

Some useful definitions and properties:

- If two vectors v_1, v_2 have vanishing scalar product $(v_1, v_2) = 0$, then they are said to be orthogonal.
- An orthogonal basis for V is a basis $\{v_1, v_2, \ldots\}$ for which $(v_i, v_j) = 0\ \forall i \neq j$. If in addition we have $(v_i, v_i) = 1\ \forall i$, then the basis is called orthonormal. In symbols we have $(v_i, v_j) = \delta_{ij}$, where δ_{ij} is the Kronecker delta: $\delta_{ij} = 1$ if $i = j$ and $\delta_{ij} = 0$ otherwise.
- The decomposition (1.1) of any vector in terms of an orthonormal basis is given by

$$v = \sum (v_i, v) v_i \quad \Rightarrow \qquad a_i = (v_i, v)\ . \tag{1.5}$$

Theorem (Schwarz inequality). Take any two vectors $v_1,\ v_2$ of a Hilbert space. Then we have

$$|(v_1, v_2)|^2 \leq ||v_1||^2 ||v_2||^2\ . \tag{1.6}$$

Proof: Consider the vector $w = v_1 + a v_2$, where a is an arbitrary complex (real) number. Then we have $||w||^2 \geq 0$, which implies

$$0 \leq ||w||^2 = (v_1, v_1) + |a|^2 (v_2, v_2) + a (v_1, v_2) + \bar{a} (v_2, v_1)\ . \tag{1.7}$$

Now we can take

$$a = -\frac{(v_2, v_1)}{(v_2, v_2)}\ . \tag{1.8}$$

In this case the last two terms of (1.7) become equal and opposite to the second one. Then we can immediately see that (1.7) reduces to (1.6).

Roughly speaking, a **Hilbert space** is a vector space with a positive definite inner product. If the vector space is infinite dimensional, we also require that:

1. The norm of each vector is finite: $\forall\ v$ we have $(v,v) < \infty$.
2. Any Cauchy sequence[2] of vectors has a limit vector in V.
3. The space has a countable orthonormal basis[3].

1.3.1 Examples and exercises.

- Consider the infinite dimensional generalization of the vectors in $\mathbf{C}^3$, that is the vectors v are just infinite arrays of complex numbers: $v = (v_1, v_2, v_3, v_4, \ldots)$. The scalar product between two vectors of this kind is defined to be $(w,v) = \sum_{k=1}^{\infty} \bar{w}_k v_k$. Thus in order to satisfy property 1, we focus only on the vectors for which $\sum_{k=1}^{\infty} |v|_k^2 < \infty$. One can show that this set of vectors forms a Hilbert space (that is property 2 and 3 are satisfied). This Hilbert space is usually named l^2.

  Exercise: Consider an set $\{v_1, v_2, \ldots\}$ of orthogonal vectors. Show that these vectors are linearly independent.

2 Linear maps.

2.1 Functions between two sets.

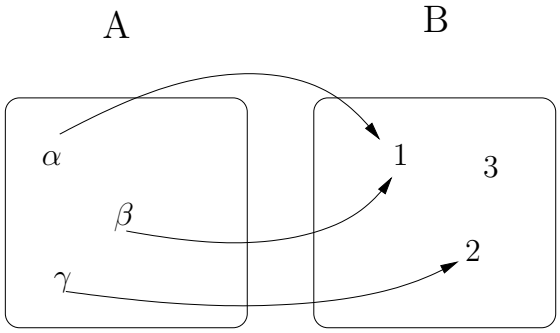
A function between two sets ($f : A \to B$) is a map that associates each element of the first set (A) one element of the second set (B). In a formal language: $\forall\ a \in A\ \exists!\ b \in B$ such that $f(a) = b$. Some definitions:

- A function $f : A \to B$ is said surjective (or "onto") if all elements of B are images of some element in A: $\forall\ b \in B\ \exists a \in A$ such that $f(a) = b$
- A function $f : A \to B$ is said injective if any two elements in A have different images in B: $\forall\ a_1, a_2 \in A\ f(a_1) = f(a_2)$ implies $a_1 = a_2$.
- a function is bijective if it is both surjective and injective.

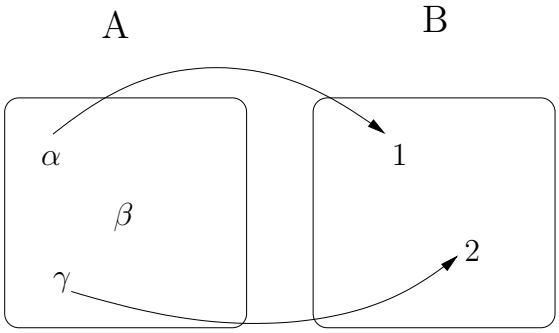
[2] A sequence of vectors v_k with $k = 1, 2, \ldots$ is Cauchy if $||v_m - v_n||^2$ becomes arbitrary small when m, n are big. In formal terms: $\forall\ \epsilon > 0\ \exists\, k \in \mathbf{N}$ such that $\forall\ m, n > k$ we have $||v_m - v_n||^2 < \epsilon$.

[3] Hilbert spaces satisfying this requirement are often called *separable*. Mathematicians consider also non-separable Hilbert spaces which satisfy the first two requirements, but not the last one; these non-separable spaces do not arise in Quantum Mechanics and so we will ignore them.

2.1.1 Examples.



This is a function.



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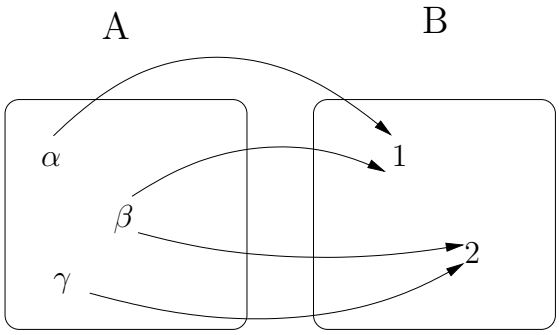

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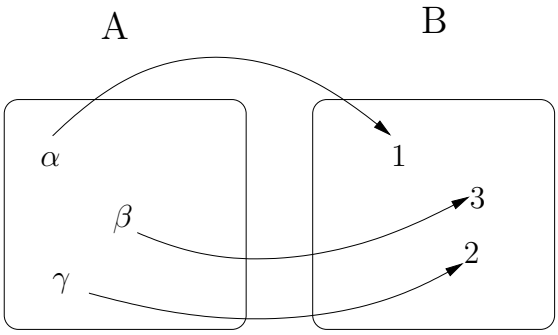


This function is bijective.

2.2 Linear functionals and Dirac's notation.

From now on we will very often indicate the vectors of an abstract vector space by using Dirac's notation $|\psi\rangle$ (*ket vector*). Depending on the type of the vector space V one is considering $|v\rangle$ can be a n-tuple of number, a polynomial or an element of l^2 (see the example in the previous Section). This notation is useful when one considers the dual space of linear functionals.

A linear functional is a function χ between a real (complex) vector space V and the real (complex) numbers which has the following property

- $\forall\ |\psi_1\rangle,\ |\psi_2\rangle \in V$ and $\forall\ a,\ b \in \mathbf{R}$ ($\mathbf{C}$) we have $\chi(a|\psi_1\rangle + b|\psi_2\rangle) = a\chi(|\psi_1\rangle) + b\chi(|\psi_2\rangle)$.

The dual space V^* is the set of all possible linear functionals. In the Dirac's notation each linear functional is represented by a $\langle\chi|$ (*bra vector*).

To every ket corresponds a bra. In a vector space with a scalar product, it is easy to define a function that maps the vectors of V into elements of V^*. For each $|\phi\rangle \in V$ consider the scalar product between $|\phi\rangle$ and any other element of V. This is a linear functional

mapping V in $\mathbf{R}$ ($\mathbf{C}$) that is completely specified by $|\phi\rangle$. Thus we can represent this linear functional with $\langle\phi|$

$$(|\phi\rangle, |\psi\rangle) \equiv \langle\phi|\psi\rangle \ . \tag{2.1}$$

From now on we will often indicate the scalar products between two vectors by using Dirac's notation, that is by using the left hand side of Eq. (2.1). Let us recall the main properties of the scalar product

$$\begin{aligned} \langle\phi|\chi\rangle &= \overline{\langle\chi|\phi\rangle} \ , \\ \langle\phi|a_1\chi_1 + a_2\chi_2\rangle &= a_1\langle\phi|\chi_1\rangle + a_2\langle\phi|\chi_2\rangle \ , \\ \langle a_1\phi_1 + a_2\phi_2|\chi\rangle &= \bar{a}_1\langle\phi_1|\chi\rangle + \bar{a}_2\langle\phi_2|\chi\rangle \ , \\ \langle\chi|\chi\rangle &> 0 \ , \quad \forall\ |\chi\rangle \neq 0 \ . \end{aligned} \tag{2.2}$$

The correspondence between ket and bra vectors is *antilinear*: if the bra vectors corresponding to $|\psi_1\rangle$ and $|\psi_2\rangle$ are $\langle\psi_1|$ and $\langle\psi_2|$, then the bra vector corresponding to $a_1|\psi_1\rangle + a_2|\psi_2\rangle$ is $\bar{a}_1\langle\psi_1| + \bar{a}_2\langle\psi_2|$

$$a_1|\psi_1\rangle + a_2|\psi_2\rangle \Rightarrow \bar{a}_1\langle\psi_1| + \bar{a}_2\langle\psi_2| \ . \tag{2.3}$$

Question: Is there a ket corresponding to every bra?
The answer is yes for finite dimensional vector spaces with a scalar product, while for infinite dimensional spaces the situation is subtler.

Let us first focus on the simple finite dimensional case. We can choose an orthonormal basis $\{|\psi_1\rangle, |\psi_2\rangle, \ldots, |\psi_n\rangle\}$ which means that we have $\langle\psi_j|\psi_i\rangle = \delta_{ij}$. For each linear functional $\langle\chi|$ we can build a vector as follows

$$\sum_{i=1}^{n} \overline{\langle\chi|\psi_i\rangle}\ |\psi_i\rangle \equiv |\chi\rangle \ . \tag{2.4}$$

Notice that the bra associated to ket just defined in (2.4) is the original linear functional $\langle\chi|$, as it can be seen by using (2.1). Proof: take any vector $|\phi\rangle$, this can be decomposed in a unique way on the basis $|\psi_i\rangle$ ($|\phi\rangle = \sum c_i|\psi_i\rangle$); then the bra associated to $|\chi\rangle$ acts as follow

$$(|\chi\rangle, |\phi\rangle) = \sum_{i=1}^{n} \langle\chi|\psi_i\rangle\ (|\psi_i\rangle, |\phi\rangle) = \sum_{i,j=1}^{n} \langle\chi|\psi_i\rangle\delta_{ij}c_j = \langle\chi|\phi\rangle \ . \tag{2.5}$$

Now the question is: what can go wrong in the case of an infinite dimensional vector space V? In this case the sum in (2.4) becomes an infinite series and the problem is that this series might not have a limit in V even if it is a combination of vectors in V. It is possible to construct an explicit example of such a situation in the case V is *not* a Hilbert space and in particular does not satisfy the second requirement in the previous notes. This example is important for our applications to Quantum Mechanics (see below the example about Dirac's delta for some more details).

2.2.1 Examples and exercises.

- Bra for finite dimensional Hilbert spaces.

Consider the space $\mathbf{C}^3$: the element of this space are just column vectors with a triplet of complex numbers (see for instance 1.2). We use the standard scalar product

$$(|v\rangle, |w\rangle) \equiv \bar{v}_1 w_1 + \bar{v}_2 w_2 + \bar{v}_3 w_3 = \begin{pmatrix} \bar{v}_1 & \bar{v}_2 & \bar{v}_3 \end{pmatrix} \begin{pmatrix} w_1 \\ w_2 \\ w_3 \end{pmatrix} \ . \tag{2.6}$$

Then, by using Eq. (2.1), it is clear that the bra corresponding to the vector $|v\rangle$ is simply the row-vector $\begin{pmatrix} \bar{v}_1 & \bar{v}_2 & \bar{v}_3 \end{pmatrix}$.

- Dirac's delta.

Consider the space of the following "nice" function $f : \mathbf{R} \to \mathbf{C}$: f is infinitely differentiable and goes to zero very quickly[4] as $|x| \to \infty$. This set of functions form a complex vector space[5] V_f with scalar product defined as

$$\int_{-\infty}^{\infty} \bar{g}(x) f(x) dx \ . \tag{2.7}$$

Consider the mapping $f(x) \to f(x = 0)$. This is a linear functional[6] that we will call $\langle \delta_0 |$. We can represent this functional by using the scalar product (2.7) and the Dirac's delta

$$\langle \delta_0 | f \rangle \equiv \int_{-\infty}^{\infty} \delta(x) f(x) dx = f(0) \ . \tag{2.8}$$

Notice that there is *no* standard function g for which $\int_{-\infty}^{\infty} \bar{g}(x) f(x) = f(0)$ for any $f(x) \in V_f$. This shows that this linear functional cannot be represented by the scalar product of an element in V, but requires a new object (the Dirac's delta in this case).

Exercise

- Prove the statement: V_f is a vector space.
- Prove the statement: $\langle \delta_0 |$ is a linear functional.

* Show explicitly that V_f is not a Hilbert space.

[4] $\forall\ n, m = 1, 2, \ldots$ we have $|x^n d^m f / dx^m| \to 0$ as $|x| \to \infty$.

[5] See the exercise below.

[6] See the exercise below.

2.3 Linear operators.

Consider two vector spaces V and W (they are not necessarily different, we can have $V = W$). A linear operator is a function A from V to W satisfying

- $\forall |\chi_i\rangle \in V$ we have $A(|a_1\chi_1 + a_2\chi_2\rangle) = a_1 A(|\chi_1\rangle) + a_2 A(|\chi_2\rangle) \in V'$

In the case $V = W$ we can define the product of two operators in a simple way just by acting on the vectors in an ordered way:

$$\forall\ \chi \in V \qquad AB(|\chi\rangle) \equiv A\Big(B(|\chi\rangle)\Big)\ .$$

Any real (complex) finite dimensional vector space V is isomorphic to $\mathbf{R}^n$ ($\mathbf{C}^n$). This means that there is a injective linear map between V and $\mathbf{R}^n$ (or $\mathbf{C}^n$).

In order to see this let us take a basis for V: $\{|v_1\rangle, \ldots, |v_n\rangle\}$. Then any vector $|v\rangle \in V$ can be decomposed along this basis

$$|v\rangle = \sum_i c^i |v_i\rangle \quad \Rightarrow \qquad \begin{pmatrix} c^1 \\ c^2 \\ \vdots \\ c^n \end{pmatrix} \leftrightarrow |v\rangle\ , \tag{2.9}$$

where c^i are the coordinates[7]. Thus we can associate to any $|v\rangle \in V$ a unique n-tuple of numbers; vice-versa to any n-tuple of numbers we can associate a vector simply be reading (2.9) in the opposite sense. Thus the map is injective. In order to complete the proof that this is an isomorphism between V and $\mathbf{R}^n$ (or $\mathbf{C}^n$), see the first exercise below.

2.3.1 Examples and exercises.

- In the case of finite dimensional vector spaces, any linear operator $A : V \to V'$ can be represented by a matrix.

In order to see this let us take a basis for V $\{|v_1\rangle, \ldots, |v_n\rangle\}$ and one for W $\{|w_1\rangle, \ldots, |w_m\rangle\}$. Then we have

$$A|v\rangle = \sum_{i=1}^{n} c^i A|v_i\rangle\ . \tag{2.10}$$

Now let us focus on each $A|v_i\rangle$: these vectors belong to W so they can be decomposed along the $|w_j\rangle$ basis

$$A|v_i\rangle = \sum_{j=1}^{m} |w_j\rangle a^j{}_i \quad \Rightarrow \qquad A|v\rangle = \sum_{i=1}^{n}\sum_{j=1}^{m} a^j{}_i c^i\ |w_j\rangle\ . \tag{2.11}$$

[7] As a notation, from now on we will use upper indices for the vector coordinates; you will see why this is convenient.

By using the isomorphism introduced above, we can

- represent the kets $|v\rangle \in V$ as column vectors with n numbers,
- represent the kets $|W\rangle \in W$ as column vectors with m numbers,
- represent the linear operator A as the matrix $a^j{}_i$, where j is the row index and i is the column index.

- A projector is a linear operator P from a vector space V to itself ($P : V \to V$) such that $P^2 = P$. This definition generalized to an abstract vector space the idea of projection in the standard Euclidean space. Dirac's notation provides a simple way to write projectors in a simple way. Consider a vector with norm 1: $|v\rangle$ and consider also the associated bra $\langle v|$. We can define a projector $P_v \equiv |v\rangle\langle v|$ which acts as follow
$$\forall\ |w\rangle \in V \quad P_v|w\rangle \equiv (\langle v|w\rangle)\ |v\rangle\ . \tag{2.12}$$
This is a projector since $P_v^2 = |v\rangle\langle v|v\rangle\langle v| = P_v$. If you take V to be, for instance, the standard 2-dimensional vector space and $|v\rangle$ to be the versor along the x-axis, then you can see that (2.12) is indeed the projection on this axis.

It is straightforward to generalize (2.12) when you deal with more vectors: if you have a set of orthonormal vectors $\{|v_1\rangle, \ldots, |v_m\rangle\}$, then you can define a projector on the plane generated by these vectors as follow
$$P_m = \sum_{i=1}^{m} |v_i\rangle\langle v_i|\ . \tag{2.13}$$

Exercise

1) Prove that the map in (2.9) is linear.
2) Consider a set of orthonormal vectors $|v_1\rangle, \ldots$ that forms a basis for V. Prove that the associated projector, as in (2.13), is the identity operator: $P = 1$.
3) Consider a finite dimensional complex Hilbert space and the isomorphism (2.9) with $\mathbf{C}^n$. Derive how the scalar product between two vectors $|v\rangle$ and $|w\rangle$ is written in terms of their coordinates.

2.3.2 Action of a linear operator on a bra.

So far we have discussed the action of linear operators on the kets in a vector space V. Let us focus on operators from V to V. By using the scalar product, it is simple to define an action also on the linear functionals (that is the bras). Consider a linear operator A, then for any bra $\langle\phi|$ we can associate a new bra $\langle\phi'|$ defined as follow

$$\forall\ |\psi\rangle \in V \qquad \langle\phi'|\psi\rangle \equiv \langle\phi|\,(A|\psi\rangle) = \langle\phi|A|\psi\rangle\ . \tag{2.14}$$

The correspondence $\langle\phi| \to \langle\phi'| \equiv \langle\phi|A$ is linear:

$$(a_1\langle\phi_1| + a_2\langle\phi_2|)A = a_1\langle\phi_1|A + a_2\langle\phi_2|A\ . \tag{2.15}$$

2.3.3 Examples.

- We have seen that in the case of a finite dimensional Hilbert space, linear operators can be represented by standard matrices. The action of an operator on a vector is then represented by the standard left multiplication of the corresponding matrix on the vector coordinates $A|v\rangle \to \sum_i a^j{}_i c^i$. The action on the bras defined above corresponds to right matrix multiplication: $\langle v|A \to \sum_j \bar{c}_j a^j{}_i$.

2.4 Hermitian and self-Adjoint operators.

Let us consider an operator A defined in a subvector space $W \subseteq V$ (of course we might have $W = V$). If for any pair of vectors $|v_1\rangle$, $|v_2\rangle \in W$ we have that $\langle Av_1|v_2\rangle = \langle v_1|Av_2\rangle$ then A is a Hermitian operator.

By using the previous paragraph A defines also a linear operator on the bras. Now, by using the bra/ket relation, we can define a new operator $A^\dagger$ on the kets ($A^\dagger$ is called the *adjoint* of A): $\forall\ |\psi\rangle \in V$ we define $A^\dagger|\psi\rangle$ as the ket corresponding[8] to the linear functional $\langle\psi|A$ acting on W. Even if this definition might seem abstract we will see that it is just the generalization of the standard Hermitian conjugation for (possibly infinite dimensional) Hilbert spaces. Let me summarize the main properties of the Adjoint operation:

$$(A+B)^\dagger = A^\dagger + B^\dagger\ , \tag{2.16}$$

$$\forall a \in \mathbf{C} \quad \Rightarrow \quad (aA)^\dagger = \bar{a}A^\dagger\ , \tag{2.17}$$

$$(A\,B)^\dagger = B^\dagger A^\dagger\ . \tag{2.18}$$

The first two properties follow from the linearity of A and B on the bra and from the antilinearity of the bra/ket relation. Eq. (2.18)

[8] There is a subtlety: there might be no corresponding ket; in this case we just eliminate $|\psi\rangle$ from the domain of $A^\dagger$.

An operator is Hermitian if $A^\dagger = A$. [Subtlety: notice that in this definition I have been vague on the domain of definition of A and $A^\dagger$. In the case of infinite dimensional spaces the domains of the two operators might be different, even if the $A^\dagger$ and A are equal on the common part of the two domains. A self-adjoint operator is an Hermitian operator for which the domains of A and $A^\dagger$ are also equal. Except for the example below, we will use the words "Hermitean" and "self-adjoint" as equivalent and asssume that there are no subtelties with the definition of the domain of the operators.].

2.4.1 Examples and exercises.

- Consider a finite dimensional Hilbert space V. We know that is isomorphic to $\mathbf{C}^n$ and that each linear operator A in V is mapped in a matrix $a^j{}_i$ in $\mathbf{C}^n$. Then Hermitian operators just correspond to Hermitian matrices. Moreover there are no subtleties with the definitions of the domains (as they always coincide with the whole vector space); then the operators corresponding to Hermitian matrices are also self-adjoint.

- In the case of infinite dimensional vector spaces, one has to pay some attention to the domain where the linear operator are defined. For instance, consider the space V of smooth functions $(\psi(x))$ in $\mathbf{R}$ which are square integrable and the operator position (x): it is not guaranteed that $x\psi(x)$ is an element of V and so x is not defined over the whole V. Example: $\psi(x) = A\frac{x}{1+x^2}$.

- A Hermitian, but not self-adjoint operator. Consider the wavefunctions you have seen in the problem of the infinite potential well

$$|n\rangle \equiv \sin\left(\frac{n\pi x}{L}\right) \ , \qquad \text{with} \ \ x \in [0, L] \ .$$

  Consider the vector space W generated by any finite linear combination of these functions with the standard scalar product $\int_0^L \bar{g}(x)\, f(x)\, dx$. Then the operator $P = -i\frac{d}{dx}$ is Hermitian, but cannot be extended to be a self-adjoint operator.

Exercise

- Prove that $\langle\phi|A^\dagger|\psi\rangle = \overline{\langle\psi|A|\phi\rangle}$ (of course suppose that $|\phi\rangle$ belongs to the domains of A and $|\psi\rangle$ to the domain of $A^\dagger$).

3 Eigenvalues and Eigenvectors.

3.1 Definition.

Let complex V be a vector space. Consider a linear operator A from V to itself $A : V \to V$. A vector $|v\rangle \in V$ that satisfy

$$A|v\rangle = \lambda|v\rangle, \tag{3.1}$$

for some complex number λ is called eigenvector and λ is called eigenvalue[9]. Of course, since A is linear, one can rescale $|v\rangle$ by an arbitrary number (as in $|v'\rangle = c|v\rangle$) and build a new eigenvector ($|v'\rangle$) with the same eigenvalue. It is also possible that a vector $|w\rangle$, that is linearly independent from $|v\rangle$, is an eigenvector with the same eigenvalue (that is we might have $A|w\rangle = \lambda|w\rangle$). It is straightforward to prove that the set of all eigenvectors with the same eigenvalue form a vector space (called eigenspace) that is a subspace of V.

[Revision from MT2/MT3]. If V is a finite dimensional vector space, we have a clear algorithm to find the eigenvalues and the eigenvectors.

- Any finite dimensional vector space V is isomorphic to $\mathbf{C}^n$ and any linear operator from V to itself can be represented as a matrix $a^j{}_i$ acting on $\mathbf{C}^n$.
- The eigenvalues are the solutions of the following equation: $\det\left(a^j{}_i - \lambda\delta^j{}_i\right) = 0$ (this is a polynomial equation whose degree is equal to the dimension of the vector space).
- For each eigenvalue we can find the corresponding eigenvector by solving the following set of n linear equations

$$\sum_{i=1}^{n} a^j{}_i c^i - \lambda c^j = 0 \ , \qquad j = 1, 2, \ldots, n \ . \tag{3.2}$$

Notice that eigenvectors with *different* eigenvalues form a set of linearly independent vectors.

3.1.1 Examples and exercises.

Exercise. Consider the following matrices as operators form $\mathbf{C}^2$ to itself

$$M = \begin{pmatrix} 1 & -i \\ 0 & 1 \end{pmatrix} \ , \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \ , \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \ , \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \ . \tag{3.3}$$

Find all possible eigenvectors and the corresponding eigenvalues for M and the σ_i's.

[9] The trivial solution $|v\rangle = 0$ is neglected and does not count as an eigenvector.

3.2 Eigenvectors of self-adjoint operators.

Let us start from the case of finite dimensional vector spaces that you studied in MT2/MT3. In this case, self-adjoint operators can be represented simply as Hermitian matrices. We have the following theorem.

> [T1] The eigenvectors of an Hermitian matrix A form a complete basis for $\mathbf{C}^n$ and the corresponding eigenvalues are always real.

(Sketch of a) Proof: the eigenvalue equation is a polynomial equation (of degree n) then it has at least one complex root (the "Fundamental theorem of algebra"). This means that there is at least one eigenvector $|v_1\rangle$. Since A is Hermitian, then A maps the space orthogonal to $|v_1\rangle$ ($V_1^\perp$) into itself: if $(|v_1\rangle, |w\rangle) = 0$ then $(|v_1\rangle, A|w\rangle) = (A|v_1\rangle, |w\rangle) = \lambda_1(|v_1\rangle, |w\rangle) = 0$. Then A restricted to $V_1^\perp$ is just a $(n-1)\times(n-1)$ matrix and we can repeat the same steps recursively to find n eigenvalues and eigenvectors. Since the eigenvectors are linearly independent, they form a basis. Notice that the basis just constructed is an *orthogonal basis*. Of course we are free to rescale the eigenvectors as we want and (3.1) is always satisfied, thus we can make the eigenvector basis *orthonormal*. So by using an exercise given in *week 2*, we can state the completeness of the eigenvectors $|v_i\rangle$ of a Hermitian matrix in the following way:

$$\sum_i |v_i\rangle\langle v_i| = 1 \ , \tag{3.4}$$

Finally notice that the eigenvalues of A are real

$$\lambda_1 ||v_1||^2 = \langle v_1, |Av_1\rangle = \langle Av_1|, v_1\rangle = \bar{\lambda}_1 ||v_1||^2 \ . \tag{3.5}$$

Now the question is what happens if we deal with self-adjoint operators defined on an infinite dimensional Hilbert space. As you can see from the example below this nice theorem cannot hold exactly in the same form. We can consider a weaker version of (3.1): look for a bra $\langle v_\lambda|$ such that

$$\langle v_\lambda|A|w\rangle = \lambda\langle v_\lambda|w\rangle \ , \tag{3.6}$$

for all $|w\rangle$ in the domain of A (λ is real, as in (3.5)). As we have seen in the example 2.2.1 on the Dirac's delta not all bras satisfying (3.6) do have a corresponding ket. Thus for a self-adjoint operator we have two cases:

- the possible eigenvalues satisfying (3.1) form a discrete set;
- the "eigenvalues" satisfying (3.6), but not (3.1), form a a continuous set.

It turns out that, even if the bras with continuous eigenvalues do not have corresponding ket, their integral over a finite region of values of λ does. In particular if $c(\lambda)$ is a smooth function that is non-zero only in a finite region of the possible λ's, then the linear functional $\int d\lambda c(\lambda)\langle v_\lambda|$ has a corresponding vector that we will indicate with $\int d\lambda c(\lambda)|v_\lambda\rangle$. With an abuse of notation, physicists commonly use also the symbol $|v_\lambda\rangle$, even if there is no $|v_\lambda\rangle$ corresponding to the bra in (3.6)! The idea is that this object yields standard vectors when integrated.

At this point we can state the infinite dimensional analogue of the theorem [T1]. Consider a self-adjoint operator: the eigenvectors $|v_i\rangle$ corresponding to discrete eigenvalues together with those related to continues eigenvalues ($|v_\lambda\rangle$) form a complete set

$$\sum_i |v_i\rangle\langle v_i| + \int d\lambda |v_\lambda\rangle\langle v_\lambda| = 1 \ . \tag{3.7}$$

The orthonormality condition reads as follow

$$\langle v_i|v_j\rangle = \delta_{ij} \quad , \qquad \langle v_{\lambda_1}|v_{\lambda_2}\rangle = \delta(\lambda_1 - \lambda_2) \ . \tag{3.8}$$

3.2.1 Examples and exercises.

- Consider the momentum operator in quantum mechanics $-i\hbar\frac{d}{dx}$ that act on differentiable, square integrable (wave)functions. There is no solution to the eigenvector equation
$$-i\hbar\frac{d\psi(x)}{dx} = \lambda\psi(x) \ . \tag{3.9}$$
It is clear that the only possibility is to choose $\psi(x) = \mathrm{e}^{\frac{i\lambda x}{\hbar}}$, but this function is not square integrable regardless whether λ is real or imaginary.

4 The postulates of quantum mechanics

1 At a fixed time t_0, the state of a physical system is defined by a vector $|\psi\rangle$ in a Hilbert space $\mathcal{H}$.

2 Every physical (measurable) quantity $\mathcal{A}$ is described by a self-adjoint operator A (also called "observable").

3 The result of a measurement of the physical quantity $\mathcal{A}$ is always one the eigenvalues of the corresponding operator A.

4 The probability of finding the eigenvalue a in a measurement is $||P_a|\psi\rangle||^2$, where $|\psi\rangle$ has unit norm and P_a is the projector on the space of eigenvectors of eigenvalue a.

5 After a measurement of $\mathcal{A}$ yielding the value a (an eigenvalue of A), then the state of the system change from $|\psi\rangle$ to $P_a|\psi\rangle/||P_a|\psi\rangle||$.

6 The time evolution of the system is described

$$H|\psi(t)\rangle = i\hbar\frac{d}{dt}|\psi(t)\rangle \ , \tag{4.1}$$

where H is the observable associated to the energy of the system (Hamiltonian).

4.0.2 Examples and exercises.

Consider the operator defined on $\mathbf{C}^3$ and the ket $|\phi\rangle$:

$$A = \begin{pmatrix} 0 & 2 & 0 \\ 2 & 0 & 0 \\ 0 & 0 & 2 \end{pmatrix} \ , \qquad |\phi\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} i \\ 0 \\ 1 \end{pmatrix} \ . \tag{4.2}$$

The operator A has the following three eigenvectors:

$$|\psi_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} \ , \quad |\psi_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix} \ , \quad |\psi_3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \ . \tag{4.3}$$

with eigenvalues 2, -2 and 2 respectively. Thus the projectors on the two eigenspaces are

$$P_{(2)} = |\psi_2\rangle\langle\psi_2| + |\psi_3\rangle\langle\psi_3| \ , \qquad P_{(-2)} = |\psi_1\rangle\langle\psi_1| \ . \tag{4.4}$$

If the state of our physical system is described by $|\phi\rangle$, then I can compute the probabilities of measuring ± 2 by decomposing $|\phi\rangle$ on the basis (4.3)

$$|\phi\rangle = P_{(2)}|\phi\rangle + P_{(-2)}|\phi\rangle = \sum_{i=1}^{3}\langle\psi_i|\phi\rangle|\psi_i\rangle \ . \tag{4.5}$$

The probability of finding -2 is $||P_{(-2)}|\phi\rangle||^2 = 1/4$, while that for 2 is $||P_{(2)}|\phi\rangle||^2 = 3/4$.

Exercise. Consider the Hilbert space $\mathbf{C}^2$ and the observable σ_1 in (3.3). If a quantum mechanical system is described by the state

$$|\psi\rangle = \begin{pmatrix} 1 \\ 2 \end{pmatrix} \ , \tag{4.6}$$

- What is the probability, in a physical measure, of finding as a result the first and the second eigenvalue?
- If the result of this measure is the positive eigenvalues, what are the possible results in a subsequent measure of the observable $\sin\theta\sigma_2 + \cos\theta\sigma_3$? What are the probabilities of finding each result?

5 Some simple quantum mechanical system.

We will focus on some simple quantum mechanical systems that have a time independent Hamiltonian. In this case it is simple to describe in general how a vector $|\psi(t_0)\rangle$, representing the system at the time t_0, evolves with time. If $\hat{H}$ is time independent, one can check that the following state

$$|\psi(t)\rangle = \mathrm{e}^{-\frac{i\hat{H}}{\hbar}(t-t_0)}|\psi(t_0)\rangle \equiv \sum_{n=0}^{\infty} \frac{1}{n!}\left[\frac{-i\hat{H}}{\hbar}(t-t_0)\right]^n |\psi(t_0)\rangle \tag{5.1}$$

solves the time evolution equation of the postulate 6. In order to compute explicitly $|\psi(t)\rangle$ it is clearly convenient to decompose $|\psi(t_0)\rangle$ along the complete basis of the Hamiltonian eigenvector. So one of the tools we need is the set of the solutions of the "time independent Schroedinger equation" $\hat{H}|\psi_E\rangle = E|\psi_E\rangle$. Often this problem can be simplified by exploiting the following observation.

Two observables $\hat{A}$ and $\hat{B}$ that commute ($[\hat{A},\hat{B}]=0$) have a common set eigenspaces. This means that we can find projectors $P_{(a,b)}$ that project at the same time on the subspace of eigenvalue a for the first operator $\hat{A}$ and the the subspace of eigenvalue b for the second operator $\hat{B}$. You can convince yourself that this is reasonable, by looking at the simple case of finite dimensional Hilbert spaces: in this case if two Hermitian matrices commute, they have a common set of eigenvectors. Sketch of a proof: Suppose that the $|v_a\rangle$ is the only eigenvector of eigenvalue a of the Hermitian matrix A. If $[A,B]=0$, it is easy to see that also $B|v_a\rangle$ is an eigenvector of A with eigenvalue a: $A(B|v_a\rangle) = BA|v_a\rangle = a(B|v_a\rangle)$. This means that $B|v_a\rangle$ must be proportional to $|v_a\rangle$, in formulae: $B|v_a\rangle = b|v_a\rangle$, which implies that $|v_a\rangle$ is also an eigenvector of B.

This means that, if we find an observable $\hat{A}$ that commute with the Hamiltonian ($[\hat{A},\hat{H}]$), then we can simplify the eigenvalue equation $\hat{H}|\psi_E\rangle = E|\psi_E\rangle$, by looking for the eigenvectors of $\hat{H}$ in each eigenspace of $\hat{A}$.

5.1 A free particle

Consider a massive particle that is free to move in one dimension. You are familiar with the quantum mechanical description of such system in terms of a (wave)function $\psi(x,t)$ and the Schroedinger equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) = i\hbar\frac{\partial}{\partial t}\psi(x,t)\ . \tag{5.2}$$

We can now see how this system fits the general framework described in the previous lectures: $\psi(x,t)$ is an element of a Hilbert space $\mathcal{F}$ of functions (see the comment below if

you are interested to know more about $\mathcal{F}$) with the scalar product defined in (2.6). The Hamiltonian is defined as

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \ . \tag{5.3}$$

Let us re-interpret this description in terms of an abstract Hilbert space, where we have a position and a momentum operator satisfying

$$[\hat{x}, \hat{p}] \equiv \hat{x}\,\hat{p} - \hat{p}\,\hat{x} = i\hbar \ . \tag{5.4}$$

We use the symbol $|x_0\rangle$ to indicate the "generalized" eigenvectors of the position operator $\hat{x}$ and $|\psi\rangle$ to indicate the ket representing the state of our system. The usual wavefunction represents nothing else than the coordinates of $|\psi\rangle$ along the basis $|x_0\rangle$

$$\psi(x_0) \equiv \langle x_0|\psi\rangle \ . \tag{5.5}$$

In this basis we have

- The position operator $\hat{x}$ is represented by the standard multiplication, that is the action of $\hat{x}$ on the vector $|\psi\rangle$ correspond to multiply the wavefunction by x.
- Then from (5.4) we see the the momentum operator is $\hat{p} = -i\hbar\frac{\partial}{\partial x}$.
- $|x_0\rangle$ is represented by $\delta(x - x_0)$ (notice that this satisfies the normalization (3.8)).

Another very convenient basis is given by the (generalized) momentum eigenvectors $|p_0\rangle$. We know that in the position basis (that is when $\hat{p} = -i\hbar\frac{\partial}{\partial x}$) we have

$$\langle x|p_0\rangle = \frac{1}{\sqrt{2\pi\hbar}}\mathrm{e}^{\frac{i}{\hbar}p_0 x} \ . \tag{5.6}$$

The factors in front has been chosen in order to satisfy the normalization condition (3.8). From (5.6) we see that the change from the coordinate basis to the momentum basis is nothing else but the Fourier transformation

$$\psi(x_0) = \int_{-\infty}^{\infty}\langle x_0|p_0\rangle\langle p_0|\psi\rangle dp_0 = \int_{-\infty}^{\infty}\mathrm{e}^{\frac{i}{\hbar}p_0 x_0}\psi(p_0)\frac{dp_0}{\sqrt{2\pi\hbar}} \ , \tag{5.7}$$

where we have defined $\langle p_0|\psi\rangle \equiv \psi(p_0)$. The inverse relation expressing $\psi(p_0)$ in terms of $\psi(x_0)$ is simply

$$\psi(p_0) = \int_{-\infty}^{\infty}\langle p_0|x_0\rangle\langle x_0|\psi\rangle dx_0 = \int_{-\infty}^{\infty}\mathrm{e}^{\frac{-i}{\hbar}p_0 x_0}\psi(x_0)\frac{dx_0}{\sqrt{2\pi\hbar}} \ . \tag{5.8}$$

For the free particle the momentum basis is convenient because we know that the free Hamiltonian is $\hat{H} = \frac{\hat{p}^2}{2m}$ and this implies that $\hat{H}$ and $\hat{p}$ commute

$$[\hat{H}, \hat{p}] = 0 \ . \tag{5.9}$$

Thus the eigenvectors (5.6) of $\hat{p}$ are also eigenvectors of $\hat{H}$. Thus we can now write the time evolution of a generic vector $|\psi(t_0)\rangle$. We first write the state in the momentum basis and then use (5.1) to obtain

$$|\psi(t)\rangle = \int_{-\infty}^{\infty} \mathrm{e}^{-\frac{ip^2}{2m\hbar}(t-t_0)} \psi(p,t_0)\, |p\rangle dp \tag{5.10}$$

Subtlety: The precise definition of $\mathcal{F}$ is subtle somewhat subtle. Of course the functions in $\mathcal{F}$ must be square integrable (the norm of the wavefunction should be finite) and, in order to show that this is really a Hilbert space, one needs to Lebesgue approach to defining the integrals. Moreover, consider two functions differ only in one point

$$f(x) = \frac{1}{1+x^2} \quad , \qquad g(x) = \begin{cases} \frac{1}{1+x^2} & \text{if} \quad x \neq 0 \\ 0 & \text{if} \quad x = 0 \end{cases} \tag{5.11}$$

Clearly we want to say that these two functions represent the same physical state, even if strictly speaking they are not equal. The "easiest" characterisation of $\mathcal{F}$ is to start with the vector space discussed in the example 2.2.1 of *week 2* notes and consider its *completion*[10]. Mathematicians refer to this Hilbert space as $L^2(-\infty, \infty)$.

5.1.1 Examples and exercises.

- Heisenberg uncertainty principle: by the triangular inequality and the commutation relation (5.4), we can derive Heisenberg's uncertainty principle. Let us suppose that the system (a massive particle in our case) is described by a $|\psi\rangle$. We can define the uncertainty on the measure of $\hat{x}$ and $\hat{p}$ has follows

$$(\Delta x)^2 = \langle\psi|(\hat{x}-x_a)^2|\psi\rangle \ , (\Delta p)^2 = \langle\psi|(\hat{p}-p_a)^2|\psi\rangle \ , \tag{5.12}$$

  where x_a (p_a) are the average values of the position (momentum): $x_a = \langle\psi|\hat{x}|\psi\rangle$. We can see that $[(\hat{x}-x_a),(\hat{p}-p_a)] = [\hat{x},\hat{p}]$. Thus by using (5.4) we see that $\langle\psi|[(\hat{x}-x_a),(\hat{p}-p_a)]\psi\rangle = i\hbar$. Then

$$\begin{aligned} \hbar^2 &= |[(\hat{x}-x_a),(\hat{p}-p_a)]\psi\rangle|^2 = |\langle(\hat{x}-x_a)\psi|(\hat{p}-p_a)\psi\rangle - \langle(\hat{p}-p_a)\psi|(\hat{x}-x_a)\psi\rangle|^2 \\ &\leq |2\langle(\hat{x}-x_a)\psi|(\hat{p}-p_a)\psi\rangle|^2 \leq 4||(\hat{x}-x_a)|\psi\rangle||^2||(\hat{p}-p_a)|\psi\rangle||^2 \ . \end{aligned} \tag{5.13}$$

  where in the last step I used Schwarz inequality (1.6).

[10] This means that we add a new element to the vector space for each different Cauchy sequence which had no limit in the original vector space; in this way the requirement 2 in the definition of a Hilbert space is satisfied by construction.

- Consider a free particle of mass m. If a certain instant ($t = 0$) the particle is detected in $x = 0$ with an experimental uncertainty a. What's the probability of finding this particle at a distance at least y from the origin at the time t? The approach you are probably familiar with is to write down Eq. (5.2) and try to find a solution for which[11]

$$\psi(x, t = 0) = \left(\frac{2}{\pi a^2}\right)^{\frac{1}{4}} \mathrm{e}^{-\frac{x^2}{a^2}} \ . \tag{5.14}$$

(recall postulate 5!). The approach described in this paragraph suggests to use the momentum basis. In this basis we have

$$\begin{aligned} \psi(p, t = 0) &= \int_{-\infty}^{\infty} \langle p|x\rangle\langle x|p\rangle dx = \left(\frac{2}{\pi a^2}\right)^{\frac{1}{4}} \int_{-\infty}^{\infty} \mathrm{e}^{-\frac{x^2}{a^2} - \frac{i}{\hbar}px} \frac{dx}{\sqrt{2\pi\hbar}} \\ &= \left(\frac{a^2}{2\pi h^2}\right)^{\frac{1}{4}} \mathrm{e}^{-\frac{a^2p^2}{4\hbar^2}} \ . \end{aligned} \tag{5.15}$$

Thus the evolved wavefunction in momentum space is

$$\psi(p, t) = \left(\frac{a^2}{2\pi h^2}\right)^{\frac{1}{4}} \mathrm{e}^{-\frac{ip^2t}{2m\hbar} - \frac{a^2p^2}{4\hbar^2}} \tag{5.16}$$

Now we can go back to position space where it is easier to compute the probability requested by the problem

$$\psi(x, t) = \left(2\pi a^2\right)^{\frac{1}{4}} \int_{-\infty}^{\infty} \exp\left(-\frac{ip^2t}{2m\hbar} - \frac{a^2p^2}{4\hbar^2} + \frac{ipx}{\hbar}\right) \frac{dp}{2\pi\hbar} \ . \tag{5.17}$$

This is again a Gaussian integral and can be explicitly evaluated to find the wavefunction in the standard position space. The result takes exactly the same form of the $t = 0$ wavefunction (5.14), just with a time depedent parameter a!

$$\psi(x, t) = \left(\frac{2f(t)}{\pi a^2}\right)^{\frac{1}{4}} \mathrm{e}^{-f(t)\frac{x^2}{a^2}} \ , \tag{5.18}$$

where $f(t)$ is a complex number and can be written as the product of its norm and phase or as the sum of the real and imaginary parts

$$f(t) = \frac{1}{1 + \frac{2\mathrm{i}\hbar t}{a^2m}} = \frac{\mathrm{e}^{\mathrm{i}\theta(t)}}{\sqrt{1 + \frac{4\hbar^2t^2}{a^4m^2}}} = \frac{1 - \frac{2m\hbar\mathrm{i}t}{a^2m^2}}{1 + \frac{4\hbar^2t^2}{a^4m^2}} \ . \tag{5.19}$$

[11] As usual, one can choose the overall constant A to work with a state of norm one: $A = (2\pi)^{1/4}\sqrt{a}$.

So finally we can write the wavefunction at the time t and, in order to keep it as simple as possible, we summarize the overall phase in $\exp(i\Theta(t))$

$$\psi(x,t) = \left(\frac{2f(t)}{\pi a^2}\right)^{\frac{1}{4}} \mathrm{e}^{\mathrm{i}\frac{2m\hbar i t}{a^2 m^2}\frac{x^2}{a^2}} \exp\left(-\frac{x^2}{a^2(1+\frac{4\hbar^2 t^2}{a^2 m^2})}\right) \ . \tag{5.20}$$

Notice that the probability density in position space is a Gaussian with a time dependent width

$$a(t) = \frac{a}{\sqrt{|f(t)|}} = a\sqrt{1+\frac{4\hbar^2 t^2}{a^4 m^2}} \ . \tag{5.21}$$

So the uncertainty on the position of the particle increases over time. Since the average position is zero, we have

$$\Delta x^2 = \int_{-\infty}^{\infty} x^2 |\psi(x,t)|^2 dx = \frac{a^2}{4}\left(1+\frac{4\hbar^2 t^2}{a^4 m^2}\right) \tag{5.22}$$

However the uncertainty over the momentum is constant! This is not immeaditely evident if we use the standard formulation

$$\Delta p^2 = \int_{-\infty}^{\infty} \psi(x,t)^*(-\hbar^2)\frac{d^2\psi(x,t)}{dx^2}dx = \frac{\hbar^2}{a^2} \ , \tag{5.23}$$

but it is obvious if we use $\psi(p,t)$ in (5.16)

$$\Delta p^2 = \int_{-\infty}^{\infty} p^2 |\psi(p,t)|^2 dp = \int_{-\infty}^{\infty} p^2 |\psi(p,t=0)|^2 dp = \frac{\hbar^2}{a^2} \ . \tag{5.24}$$

Exercise. Consider a particle of mass m that is constrained to be in a 1-dimensional box of size $2a$, but that otherwise is free. For sake of concreteness, we will parametrize the box with $-a < x < a$.

- Find the eigenvectors and the eigenvalues of the Hamiltonian describing this system.
- At the time $t = 0$, the particle is described by the wavefunction $\psi(t = 0)$ which is in the positive half of the box ($0 < x < a$) with equal probability of being in any point of that part of the box. What is the probability of finding, in a physical measurement at the time $t = 0$, the lowest possible eigenvalue of the energy operator?
- Consider again the wavefunction $\psi(t = 0)$ described above: calculate the wavefunction at the time t supposing that it evolves freely (that is without any external perturbation).
- What is the probability of finding the particle in the negative half of the box at the time t?

- What is the probability of finding, in a physical measurement at the time t, the lowest possible eigenvalue of the energy operator? What is the wavefunction describing the particle after this measurement?

5.2 The harmonic oscillator.

A particle of mass m moves in 1-dimension with a potential $U(x) = \frac{1}{2}kx^2$. The classical trajectory is an oscillatory motion with frequency ω

$$x(t) = A\cos(\omega t + \phi) \ , \quad \text{with} \ \ \omega = \sqrt{\frac{k}{m}} \ , \tag{5.25}$$

where ϕ is an arbitrary constant that we can set to zero by choosing an appropriate initial time $t = 0$ and A is the amplitude of the oscillation.

Quantum mechanically we know that the harmonic oscillator cannot have zero total energy, as this would violate Heisenberg's uncertainty principle. The state with minimal energy is called ground state and has energy $E_0 = \hbar\omega/2$. Then we have an infinite set of excited states with energies $E_n = \hbar\omega(n + 1/2)$. Let us derive these results by using an abstract operator description. The Hamiltonian of the system is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 \tag{5.26}$$

and we want to find the eigenvectors of $\hat{H}$. The easiest approach is to consider the operators

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} + i\sqrt{\frac{1}{2m\hbar\omega}}\hat{p} \ , \quad \hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} - i\sqrt{\frac{1}{2m\hbar\omega}}\hat{p} \ . \tag{5.27}$$

We can invert these relation and write the operators $\hat{x}$, $\hat{p}$ in terms of the lowering and raising operators

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a} + \hat{a}^\dagger\right) \ , \quad \hat{p} = -i\sqrt{\frac{m\hbar\omega}{2}}\left(\hat{a} - \hat{a}^\dagger\right) \tag{5.28}$$

In terms of the raising/lower operators the canonical commutation relations $[\hat{x}, \hat{p}] = i\hbar$ and the Hamiltonian (5.26) read

$$[\hat{a}, \hat{a}^\dagger] = 1 \ , \quad \hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right) \tag{5.29}$$

From this equation we immediately see that all energy eigenvalues must be positive. Suppose that $|\phi\rangle$ is an eigenvector of norm one and eigenvalue λ, then

$$\lambda = \langle\phi|\hat{H}|\phi\rangle = \hbar\omega\left(\langle\hat{a}\phi|\hat{a}\phi\rangle + \frac{1}{2}\right) > 0 \ . \tag{5.30}$$

An explicit realisation of the commutation relations in Eq. (5.29) is to think about the operators $\hat{a}$ and $\hat{a}^\dagger$ as acting on the space of polynomials $P(a)$ with complex coefficients: $\hat{a}$ is identified with the derivative $\frac{d}{da}$ and so it lowers the degree of the polynomial by one, while $\hat{a}^\dagger$ is identified with the multiplication by a and so raised the degree of the polynomial by one. We can easily check that this identification is consinsten with the commutation relation

$$[\hat{a}, \hat{a}^\dagger]|v\rangle = |v\rangle \quad \Leftrightarrow \qquad \frac{d}{da}\left(aP(a)\right) - a\frac{d}{da}\left(P(a)\right) = P(a) \ . \tag{5.31}$$

Then we need to define a scalar product on the space of polynomial such that the $\hat{a}$ and $\hat{a}^\dagger$ are actually one the adjoint of the other. Clearly this has to exchange the role of the multiplication by a and the derivative with the respect to a. So if each ket-vector is represented by standard polynomials (for instance $|P\rangle = a^2 + i$), the corresponding bra-vector is represented by the same polynomial where each a is substituted with a derivative and the new coefficients are the complex conjugate of the original one ($\langle P| = \frac{d^2}{da^2} - i$). The action of any bra on a vector is obtained simply be computing the action of the derivatives on the polynomial and then setting a to zero. So for instance, the scalar product of $|P\rangle$ and $|Q\rangle = a + 1$ is

$$\langle P|Q\rangle = \left[\left(\frac{d^2}{da^2} - i\right)(a+1)\right]_{a=0} = \left[\frac{d^2 a}{da^2} + \frac{d^2 1}{da^2} - ia - i\right]_{a=0} = -i \ . \tag{5.32}$$

Now it is straightforward to check that the polynomial of degree zero $|0\rangle$ is the eigenstate of $\hat{H}$ with minimal eigenvalue. In order for this to happen the first term on the right hand side of (5.30) should minimal possible value, *i.e.* zero:

$$\hat{a}|0\rangle = \left[\frac{d}{da}P(a)\right]_{a=0} = 0 \quad \Rightarrow \quad P(a) = \text{const} \ , \tag{5.33}$$

and so the corresponding eigenvalue of the harmonic oscillator Hamiltonian is $\hbar\omega/2$. By using the scalar product defined above we immediately see that the ground state as defined is normalised to one if we take $P(a) = 1$. Then it is clear that any other monomial $|n\rangle = C_n a^n$ is an eigenstate of the Hamiltonian in (5.29)

$$\hat{a}^\dagger\hat{a}|n\rangle = a\frac{d}{da}C_n a^n = nC_n a^n \ , \tag{5.34}$$

which implies that the corresponding eigenvalue for $\hat{H}$ is

$$\lambda_n = \hbar\omega\left(n + \frac{1}{2}\right) \ .$$

Again it is easy to fix the normalisation C_n by requiring

$$\langle n|n\rangle \Leftrightarrow |C_n|^2 \left[\frac{d^n}{da^n} a^n\right]_{a=0} = n!|C_n|^2 \ , \tag{5.35}$$

which implies $C_n = 1/\sqrt{n!}$. Thus we can summarise the spectrum of $\hat{H}$ by writing

$$|n\rangle = \frac{1}{\sqrt{n!}} \left(\hat{a}^\dagger\right)^n |0\rangle \ . \tag{5.36}$$

We saw that the operators operators $\hat{a}$ and $\hat{a}^\dagger$ lower/raise the energy level of an eigenstate of the Hamiltonian and that the normalised eigenvectors are related by

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle \quad \text{and} \quad \hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle \ . \tag{5.37}$$

Finally a remark on the structure of the space of the possible states for the harmonic oscillator: the space of polynomials with the scalar product defined in (5.32) is not a Hilbert space, because it does not meet the second requirement listed at the end of Section 1. Thus we need to consider its completion, that is series, and not just polynomials, in a whose coefficients are square summable. So the full space of states is isomorphic to l^2 as deined in Section 1.

5.3 Connection with the usual wavefunctions.

Let us see that there is just a single state satisfying this condition. In order to do this, it is convenient to go back to the position space description $\psi_0(x) \equiv \langle x|0\rangle$, where the condition (5.33) reads as

$$\left(\sqrt{\frac{m\omega}{2\hbar}}x + \hbar\sqrt{\frac{1}{2m\hbar\omega}}\frac{d}{dx}\right)\psi_0(x) = 0 \ . \tag{5.38}$$

This is a first order differential equation which has only one solution

$$\psi_0(x) = A\exp\left(-\frac{1}{2}\frac{m\omega}{\hbar}x^2\right) \ . \tag{5.39}$$

As usual, it is convenient to fix the overall normalization by requiring that the eigenstate has norm one, which implies

$$A = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \ . \tag{5.40}$$

We can now use again the commutation relation (5.29) and build the entire spectrum of the harmonic oscillators (that is all the eigenvectors of $\hat{H}$) from the ground state by acting with $\hat{a}^\dagger$:

$$\hat{a}|0\rangle = 0 \ \Rightarrow \quad \hat{N}\left(\hat{a}^\dagger\right)^n|0\rangle = n\left(\hat{a}^\dagger\right)^n|0\rangle \ . \tag{5.41}$$

This means that $\left(\hat{a}^\dagger\right)^n|0\rangle$ is proportional to $|n\rangle$; in particular, if we want to keep working with orthonormal eigenstates, we have

5.3.1 Examples and exercises.

Semiclassical states. The quantum mechanical energy eigenstates of the harmonic oscillator seems to be rather different from classic trajectories derived in (5.25). We would like to find a quantum mechanical state describing a motion that is very close to the classical one. In particular, we would like to find a state $|\alpha\rangle$ for which the *average* value of the position operator:

$$\langle\alpha|\hat{x}|\alpha\rangle = A\cos(\omega t+\phi) = \frac{1}{2}\left(A\mathrm{e}^{i\phi}\mathrm{e}^{i\omega t} + A\mathrm{e}^{-i\phi}\mathrm{e}^{-i\omega t}\right) \ . \tag{5.42}$$

By using (5.28), we can rewrite Eq. (5.42) as

$$\langle\alpha|\hat{x}|\alpha\rangle = \sqrt{\frac{\hbar}{2m\omega}}\langle\alpha|\hat{a}\alpha\rangle + \sqrt{\frac{\hbar}{2m\omega}}\langle\alpha|\hat{a}^\dagger\alpha\rangle \ \ . \tag{5.43}$$

Clearly if we can find a ket that is an eigenstate of $\hat{a}$ of eigenvalue

$$\alpha = \sqrt{\frac{m\omega}{2\hbar}}A\mathrm{e}^{-i\phi} \ ,$$

then (5.42) at $t=0$ would follow. So let us look for a state $|\alpha\rangle$ satisfying

$$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle \ . \tag{5.44}$$

We can use the explicit realisation of the raising and lowering operators in (5.31) and transform (5.44) in a simple differential equation

$$\frac{d}{da}f(a) = \alpha f(a) \quad \Rightarrow \qquad f(a) = \mathcal{A}\mathrm{e}^{\alpha a} \ . \tag{5.45}$$

This function is not a polynomial, but can be approximated arbitrary well by a Cauchy series of polynomials, so it is part of the l^2 space describing the Harmonic oscillator states. Thus, in abstract terms, we see that the eigenstates we are looking for are

$$|\alpha\rangle = \mathcal{A}\mathrm{e}^{\alpha\hat{a}^\dagger}|0\rangle \ . \tag{5.46}$$

These states are called coherent states and the average value for the position operator $\hat{x}$ when the state of the particle is described by the coherent state α agrees with (5.42) for any t. We can check this explicitly by evolving $|\alpha\rangle$ at a generic time

$$|\alpha,t\rangle = \mathrm{e}^{-\frac{i}{\hbar}Ht}|\alpha\rangle = \sum_{n=1}^{\infty}\mathrm{e}^{-i\omega t(n+\frac{1}{2})}\frac{\alpha^n}{\sqrt{n!}}|n\rangle \ . \tag{5.47}$$

$$\begin{aligned}\langle\alpha,t|\hat{x}|\alpha,t\rangle &= |\mathcal{A}|^2\sqrt{\frac{\hbar}{2m\omega}}\sum_{n,k=1}^{\infty}\frac{\bar{\alpha}^k\alpha^n}{\sqrt{k!n!}}\left(\mathrm{e}^{i\omega t(k-n)}\langle k|a|n\rangle+\mathrm{e}^{i\omega t(k-n)}\langle k|a^\dagger|n\rangle\right)\\ &= \frac{1}{2}\left(A\mathrm{e}^{i\phi}\mathrm{e}^{i\omega t}+A\mathrm{e}^{-i\phi}\mathrm{e}^{-i\omega t}\right)\ . \qquad (5.48)\end{aligned}$$

The second line follows from the first one by using (5.37), the result of the exrcise below for $\mathcal{A}$ and $\langle k|n\rangle=\delta_{kn}$ (recall that eigenstates with different eigenvalues are orthogonal).

Observation. There is a simpler way to derive (5.48) from (5.43). Suggestion: try to calculate the time derivative of $\langle\alpha,t|\hat{x}|\alpha,t\rangle$ by using (5.1).

Exercises.

- Normalize to one the coherent states (5.46).
- Consider a charged harmonic oscillator in a uniform constant electric field. Write the Hamiltonian and find the eigenvalues.

6 Perturbation theory.

We saw that finding the complete set of eigenvectors of the Hamiltonian is the key point to solve the dynamics of a physical system. Unfortunately it is often very difficult to solve exactly this problem. By now you have already seen the important situations where we can find all solutions to the eigenvector equation $H|\psi\rangle=E|\psi\rangle$

- The free particle and some simple variation where the potential is piecewise constant.
- The harmonic oscillator.
- A particle in a central potential $V(r)=C/r$, where C is a constant (such as the electron in the Hydrogen atom).

How can we deal with more complicated cases? Is there any hope to tackle physical interesting situations? In this section we will focus on systems that are very "close" to the simple cases that we can solve exactly, while in the next section we will consider systems with more than one constituents (multiparticle systems).

6.1 Time independent perturbation theory.

Consider a system described by an Hamiltonian H which can be splitted in two terms: H_0 that yields the dominant contribution to the energy eigenvalues and a perturbation

term δH. Suppose that we can solve exactly the eigenvalue problem for H_0 and that its spectrum of eigenvector is discrete and non-degenerate

$$H_0|\psi_n^{(0)}\rangle = E_n^{(0)}|\psi_n^{(0)}\rangle \quad \text{with} \quad n = 1, 2, \dots \tag{6.1}$$

We can solve the complete eigenvalue problem $H|\psi_n\rangle = E|\psi_n\rangle$ in an iterative approach where we treat δH in $H = H_0 + \delta H$ as a small perturbation.

With this approximation, it is intuitively clear that the exact eigenvectors $|\psi_n\rangle$ are not too different from the eigenvectors of H_0 ($|\psi_n^{(0)}\rangle$). As a guess (ansatz) we can take the exact energy E to be close to the unperturbed one

$$E_n = E_n^{(0)} + E_n^{(1)} + E_n^{(2)} + \dots \tag{6.2}$$

with $E_n^{(0)} \gg E_n^{(1)} \gg \dots$ and we can write $|\psi_n\rangle$ as

$$|\psi_n\rangle = |\psi_n^{(0)}\rangle + |\psi_n^{(1)}\rangle + |\psi_n^{(2)}\rangle + \dots \tag{6.3}$$

where $|\psi_n^{(n)}\rangle$ are smaller and smaller corrections (that is $|||\psi_n^{(2)}\rangle||^2 \ll |||\psi_n^{(1)}\rangle||^2 \ll 1$). From now let us indicate the perturbation term δH with $W^{(1)}$ in order to stress that it is of the same order of the first correction to the eigenvector (i.e. $|\psi_n^{(1)}\rangle$). By using (6.3) in the exact eigenstate equation we get

$$H_0|\psi_n^{(0)}\rangle + \big(H_0|\psi_n^{(1)}\rangle + W^{(1)}|\psi_n^{(0)}\rangle\big) + \dots = E_n^{(0)}|\psi_n^{(0)}\rangle + \big(E_n^{(0)}|\psi_n^{(1)}\rangle + E_n^{(1)}|\psi_n^{(0)}\rangle\big) + \dots \,, \tag{6.4}$$

where I we stopped to the first order in the perturbative expansion, which means that all terms of order two are understood in the dots. The first terms in the left and the right hand sides of (6.4) are equal by construction. Then we can exploit the fact that the eigenvectors $|\psi_n^{(0)}\rangle$ form a orthonormal basis and derive from (6.4)

$$\langle\psi_k^{(0)}|H_0|\psi_n^{(1)}\rangle + \langle\psi_k^{(0)}|W^{(1)}|\psi_n^{(0)}\rangle = E_n^{(0)}\langle\psi_k^{(0)}|\psi_n^{(1)}\rangle + E_n^{(1)}\delta_{kn} \,. \tag{6.5}$$

If we focus on the case $k = n$, then the first terms in the left and the right hand sides are equal. and Eq. (6.5) implies

$$E_n^{(1)} = \langle\psi_n^{(0)}|W^{(1)}|\psi_n^{(0)}\rangle \,. \tag{6.6}$$

On the other hand if we consider the case $k \neq n$ in (6.5), we can derive the form of $|\psi_n^{(1)}\rangle$

$$|\psi_n^{(1)}\rangle = \sum_{k\neq n} \frac{\langle\psi_k^{(0)}|W^{(1)}|\psi_n^{(0)}\rangle}{E_n^{(0)} - E_k^{(0)}}|\psi_k^{(0)}\rangle \tag{6.7}$$

A similar procedure can be repeated in an iterative fashion. If we now consider the second order terms in (6.4), that is the first terms that were neglected we have

$$H_0|\psi_n^{(2)}\rangle + W^{(1)}|\psi_n^{(1)}\rangle = E_n^{(0)}|\psi_n^{(2)}\rangle + E_n^{(1)}|\psi_n^{(1)}\rangle + E_n^{(2)}|\psi_n^{(0)}\rangle \,.$$

Again by taking the scalar product with $|\psi_n^{(0)}\rangle$ of this identity we get the second order correction for the energy

$$E_n^{(2)} = \sum_{k\neq n} \frac{|\langle\psi_k^{(0)}|W^{(1)}|\psi_n^{(0)}\rangle|^2}{E_n^{(0)} - E_k^{(0)}} \ . \tag{6.8}$$

A similar approach can be applied also in the case where the eigenvectors of H_0 are degenerate. In this case, one has a freedom in choosing the eigenvector basis for H_0 and the most convenient choice is to diagonalize the perturbation in each of the eigenspaces of H_0. Also the case of system] with a continuous spectrum can be treated along the same lines Please, for both these cases, refer to the books for a more detailed treatment.

6.1.1 Examples and exercises.

Consider a physical system that is described by the Hilbert space $\mathbf{C}^3$ and by the Hamiltonian

$$H = \begin{pmatrix} 4 & 2\epsilon & 0 \\ 2\epsilon & 0 & \epsilon \\ 0 & \epsilon & -1 \end{pmatrix} = \begin{pmatrix} 4 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} + \begin{pmatrix} 0 & 2\epsilon & 0 \\ 2\epsilon & 0 & \epsilon \\ 0 & \epsilon & 0 \end{pmatrix} \equiv H_0 + W^{(1)} \ .$$

The eigenvalues and eigenvectors can be easily found exactly by looking for the solution of

$$4x + 5\epsilon^2 x + 3x^2 - x^3 = 0 \ ,$$

which yields

$$x_1 = \frac{3}{2} + \frac{5}{2}\sqrt{1 + \frac{4}{5}\epsilon^2} \ , \quad x_2 = 0 \ , \quad x_3 = \frac{3}{2} - \frac{5}{2}\sqrt{1 + \frac{4}{5}\epsilon^2} \ . \tag{6.9}$$

Let us now use the approximate approach discussed in this section and treat $W^{(1)}$ as a perturbation. This is justified when $\epsilon \ll 1$, thus we should find the Taylor expansion of the results (6.9) for small ϵ . This is indeed the case. The eigenvectors of H_0 are

$$|v_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \ , \quad |v_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \ , \quad |v_3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \ , \tag{6.10}$$

with eigenvalues 4, 0, and -1 respectively. Now it is clear that, in this case, $\langle v_i|W^{(1)}|v_i\rangle = 0$, thus Eq. (6.6) implies that there are no first order corrections to the energies, in agreement with (6.9). At the following order, from (6.8) we have

$$x_1 = 4 + \epsilon^2 \ , \quad x_2 = 0 \ , \quad x_3 = -1 - \epsilon^2 \ , \tag{6.11}$$

again in agreement with the expansion of Eq. (6.9).

Exercises.

- Use perturbation theory to compute the eigenstate of H in the example above up to the first order in ϵ. Compare the results you obtained with the exact expression.
- Consider a harmonic oscillator of frequency ω perturbed by a small linear potential $W^{(1)} = \epsilon\omega\sqrt{\hbar\omega m}\hat{x}$. Use perturbation theory to find the first order corrections to the eigenvectors and the second order corrections to the eigenvalues.

7 Multiparticle systems.

So far we mainly focused on the dynamics of a single particle, but clearly we would like to apply the Quantum Mechanics formalism to more complex systems: for instance, the scattering of two particles in an accelerator, the description of atoms with more than one electrons, the descriptions of crystals etc.

7.1 Non identical particles.

The simplest situation is to consider two different particles (such as an electron and a muon). If the state of the first particle alone is described by the Hilbert space $\mathcal{H}_1$ and the state of the second one by $\mathcal{H}_2$, a physical system composed by the two particles is described by a vector in $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$, the tensor product of the two Hilbert spaces.

Already in this simple case, we can see a peculiar property of the quantum mechanical treatment of multiparticle states. We can separate the states in the tensor product space $\mathcal{H}$ in two classes

- separable states $|\psi\rangle_s$ which can be written as products of a state $|\psi\rangle_1$ in $\mathcal{H}_1$ and a state $|\psi\rangle_2$ in $\mathcal{H}_2$
- entangled states $|\psi\rangle_e$ which in any basis are described only by *sums* of products states.

In the second type of states there is a statistical correlations between measurements performed on the two particles that is peculiar to quantum mechanics. See below for an explicit example.

7.1.1 Examples and exercises.

Consider a first particle whose state is describe by the Hilbert space $\mathbf{C}^2$ and a second one whose state is in $\mathbf{C}^3$. The vectors describing the composite systems live in $\mathbf{C}^2 \otimes \mathbf{C}^3$. This is a space of dimension 6 and we can find an orthonormal basis just by multiplying the elements of the basis of the two constituents

$$|v_1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \ , \ |v_2\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \ , \ |v_3\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \ , \tag{7.1}$$
$$|v_4\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \ , \ |v_5\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \ , \ |v_6\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \ .$$

Each one of these states is clearly separable, since it is explicitly written as a product state. Thus there is no correlation between the measurements performed on each particle. For instance, we can consider the observables:

$$O_1 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \ , \quad O_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \ . \tag{7.2}$$

where O_1 acts on the first particle and O_2 on the second one. If the state of the composite system is described by $|v\rangle_1$, then the results of a measurements of both O_1 and O_2 is always yield 1. Let us now consider a different state of the composite system described by

$$\frac{1}{\sqrt{2}}\Big(|v\rangle_1 + |v\rangle_6\Big) \ . \tag{7.3}$$

This is an entagled state. The measurement of the two observables O_1 and O_2 is now related: if we carry first the measurement on the first particle and this yields the values 1 then any subsequent measurement of O_2 will also lead to the values 1. On the contrary, if the value of O_1 turns out to be -1, then also the value of O_2 in any subsequent measurement will be -1.

Exercises.
Consider the example discussed above: is the state below an entagled state?

$$\frac{1}{\sqrt{2}}\Big(|v\rangle_1 + |v\rangle_4\Big) \ . \tag{7.4}$$

7.2 Identical particles.

If we deal with a system whose constituents are identical objects then there is a further twist that is again peculiar to Quantum Mechanics. Consider a system with two identical particles that live in the same region of space (that is the wavefunctions do overlap). In a first measurement, at $t = 0$, we detect one particle in the position x_1 and the other one in the position x_2. In a second measrement at a slightly later time t, a particle is detected in the position $x_1 + \epsilon$ and another one is detected in $x_2 + \epsilon$, where ϵ is a small displacemente as $t \to 0$. In classical physics, we could follow the trajectories of each particle and say that the first one has moved from x_1 to $x_1 + \epsilon$. In Quantum Mechanics there is no way to be sure that the particle detected in $x_1 + \epsilon$ is the same as the one detected in x_1 (recall the time evolution derived in (5.20)!).

This inability to distinguish identical particle must be accounted for in the basic postulates. For instance, consider a system of two identical particles each one described by a state in the Hilbert space $\mathcal{H}$. We know that the composite system is described by a state in the tensor product $\mathcal{H}_P = \mathcal{H} \otimes \mathcal{H}$, where the two factors must be identical since the particles are identical. Since it is arbitrary to say that the first factors describes the first particle, we must require that all measurements should yield the same results even if we swap the roles of the two factors in $\mathcal{H}_P$. Of course, this can be achieved by requiring that the state $|v\rangle \in \mathcal{H}_p$ is invariant under the exchange of the two factors

$$|v\rangle = \sum_{ij} c^{ij} |v_i\rangle \otimes |v_j\rangle = \sum_{ij} c^{ij} |v_j\rangle \otimes |v_i\rangle = P^{12}|v\rangle \ , \tag{7.5}$$

where P^{12} is an operator acting on $\mathcal{H}$ that permutes the role of the two factors. However this is too restrictive, since we know that an overall phase in the state does not yield any observable consequence. In particular, for particles that propagates in more than two dimensions we can have only two cases[12]

- Bosonic particles, whose wavefunction must be symmetric $|v\rangle_B = P^{12}|v\rangle_B$.
- Fermionic particles, whose wavefunction must be antisymmetric $|v\rangle_F = -P^{12}|v\rangle_F$.

Also the observables in composite systems with identical particles must have special properties under the exchange of the labels indicating the various particles. In particular, an observable O must commute with the operation that permute the role of two particles P^{ij}: $[O, P^{ij}] = 0$, $\forall ij$.

[12] In 2-dimensional systems we can have "anyonic" particles whose symmetry properties involve an arbitrary phase.

7.2.1 Examples and exercises.

Consider a system of two identical particles each one described by a state in $\mathbf{C}^2$. If this particles are boson then the possible states are

$$|v_1\rangle_B = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} \ , \ |v_3\rangle_B = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{7.6}$$

$$|v_2\rangle_B = \frac{1}{\sqrt{2}} \left[\begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} \right] .$$

On the other hand, if the two particles are fermions then there is only one possible state

$$|v\rangle_F = \frac{1}{\sqrt{2}} \left[\begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} - \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} \right] . \tag{7.7}$$

Exercises.

- Consider a two particle state whose constituents are bosons. The initial state of the system is then described by a symmetric state. Is this property preserved by the time evolution? Why?

8 Symmetries.

We saw that Hermitean operators play a central role in Quantum Mechanics: they represent the observables of a physical system. There is another very important class of operators: the unitary operators U, that are the operators preserving the norm of any vectors

$$||U|\psi\rangle||^2 = ||\langle\psi|U^\dagger U\psi\rangle = |||\psi\rangle||^2 \ , \quad \forall|\psi\rangle \ . \tag{8.1}$$

This implies that $U^\dagger U = 1$. If we work with a finite dimensional Hilbert space, where we can represent the operators with matrices, then we can check explicitly if a matrix is unitary (see the example below). Unitary operators are important in QM, because they represent the action of a symmetry operation on a physical system: starting with a system described by the ket $|\psi\rangle$, we can obtain the ket $U|\psi\rangle$ which describes the same system after the symmetry operation related to U. U must be a unitary operator since we want to keep the normalization condition $|||\psi\rangle||^2 = 1$.

It is easy to build explicitly unitary operators starting from the Hermitean ones we have been using so far. We can just repeat the trick we used in (5.1) with the Hamiltonian: if now H is any operator satisfying $H = H^\dagger$, then we can repeat the same steps[13] and prove that $U_a = \exp(\mathrm{i}aH)$ is a unitary operator for any real a.

[13] Starting from a vector $|\psi\rangle$ of norm 1, we can check that the norm of $U_a|\psi\rangle$ is independet of a and thus is one.

8.1 Translations.

Consider a free particle in one dimension whose state is encoded by the wavefunction (5.14), which describes a particle around the position $x = 0$ with a precision determined by a. Since the particle is free, we can displace it by x_0 (so that the Gaussian is centred in x_0 instead of z_0) and many observables, such as the energy of the system, should not change. The operator representing this operation should act on (5.14) as follows:

$$U_{T(x_0)} \left[\frac{A}{\sqrt{\pi}a} \mathrm{e}^{-\frac{x^2}{a^2}} \right] = \frac{A}{\sqrt{\pi}a} \mathrm{e}^{-\frac{(x-x_0)^2}{a^2}} \ . \tag{8.2}$$

We can derive the form of $U_{T(x_0)}$ looking at the case of an infinitesimal translation (a very small x_0), so that we can Taylor-expand the right hand side of the above equation and keep only the first two terms

$$U_{T(x_0)} \left[\frac{A}{\sqrt{\pi}a} \mathrm{e}^{-\frac{x^2}{a^2}} \right] = \frac{A}{\sqrt{\pi}a} \mathrm{e}^{-\frac{x^2}{a^2}} + x_0 \frac{d}{dx_0} \left[\frac{A}{\sqrt{\pi}a} \mathrm{e}^{-\frac{(x-x_0)^2}{a^2}} \right]_{x_0=0} + \dots \ . \tag{8.3}$$

From this result we see that $U_{T(x_0)} = 1 + x_0 d/dx_0 + \ldots = 1 - x_0 d/dx + \ldots$. Thus, for small x_0 we can write $U_{T(x_0)} = 1 - \mathrm{i} x_0 \hat{p}/\hbar + \ldots$ and by using the observation above we can readily guess that

$$U_{T(x_0)} = \exp\left(-\frac{\mathrm{i}}{\hbar} x_0 \hat{p} \right) \ . \tag{8.4}$$

At this point it is easy to see that all possible translation operators form a group (see the first Section):

$$U_{T(x_0)} U_{T(x_1)} = \exp\left(-\frac{\mathrm{i}}{\hbar} x_0 \hat{p} \right) \exp\left(-\frac{\mathrm{i}}{\hbar} x_1 \hat{p} \right) = \exp\left(-\frac{\mathrm{i}}{\hbar} (x_0 + x_1) \hat{p} \right) \equiv U_{T(x_0+x_1)} \ . \tag{8.5}$$

With these results we established an important fact

> The momentum is directly related to the translation operation (technically speaking: the momentum is the generator of the translations).

Notice that, if an observable O commutes with $\hat{p}$, then the results of a measurment of O are the same if carried out on the system before or after a translation. For instance, in the case of a free particle we have $[H, \hat{p}] = 0$; then the wavefunctions (5.14) and (8.2) yields the same results for a measurement of the energy.

8.1.1 Examples and exercises.

Notice that the result (8.4) is not tight to a particular realization of the position/momentum operators, such as the position-space wavefunction. For instance, when the translation

operator acts on the momentum-space wavefunctions (see, for instance, Eq. (5.16)), then it simply multiplies $\psi(p)$ by the phase $\exp(-\mathrm{i}x_0 p/\hbar)$.

Exercises.

- Use the explicit form of the translation operator (8.4) and prove Eq. (8.2).

8.2 The rotations.

Another relevant group of symmetries is represented by the rotations (here we focus on the rotation in the 3-dimensional space). The generator of the rotation is another very important observable: the angular momentum.

$$\begin{aligned} L_x &= \hat{y}\hat{p}_z - \hat{z}\hat{p}_y \equiv L_1 \ , \\ L_y &= \hat{z}\hat{p}_x - \hat{x}\hat{p}_z \equiv L_2 \ , \\ L_z &= \hat{x}\hat{p}_y - \hat{y}\hat{p}_x \equiv L_3 \ . \end{aligned} \tag{8.6}$$

By using the canonical commutation relation $[\hat{x},\hat{p}] = \mathrm{i}\hbar$, we obtain the following relations

$$[L_1, L_2] = \mathrm{i}\hbar L_3 \quad , \qquad [L_1, L_3] = -\mathrm{i}\hbar L_2 \qquad \text{and cyclical permutations.} \tag{8.7}$$

If we repeat the same argument discussed in the case of translation, we should see that the unitary operators generated by the exponential of the angular momentum represent the rotations, that is for a rotation of an angle θ around the z-axis we should have

$$U_{R(\theta)} \mathrm{e}^{-\frac{(\vec{r}-\vec{r}_0)^2}{a^2}} = \exp\left(-\frac{\mathrm{i}}{\hbar}\theta L_z\right) \mathrm{e}^{-\frac{(\vec{r}-\vec{r}_0)^2}{a^2}} = \mathrm{e}^{-\frac{(\vec{r}-\vec{r}_1)^2}{a^2}} \ , \tag{8.8}$$

where I neglected the overall normalization of the wavefunction that is irrelevant in this computation. The position of the particle before the rotation is $\vec{r}_0$, while after the rotation is $\vec{r}_1$. The coordinates of these two points are related as explained in the example below. It is straightforward to check that (8.8) holds in the case of very small angles θ: again, as in the computation done before for the translations, it is sufficient to Taylor-expand all θ-dependent quantitites up to the first order and, in this case, use the definition of L_z, see Eq. (8.6). Notice that the wavefunctions that depend only r^2 (such as the one above with $\vec{r}_0 = 0$) are *invariant* under rotations, as expected! In order to check this it is sufficient to calculate the action of the L_i's on a (wave)function that depends only on r^2 and see that is trivial (zero). For instance

$$\begin{aligned} L_z\psi(r^2) &= -\mathrm{i}\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\psi(r^2) \\ &= -\mathrm{i}\hbar\frac{d\psi(r^2)}{dr^2}\left(x\frac{\partial r^2}{\partial y} - y\frac{\partial r^2}{\partial x}\right) = -\mathrm{i}\hbar\frac{d\psi(r^2)}{dr^2}\left(2xy - 2yx\right) = 0 \ . \end{aligned} \tag{8.9}$$

A similar computation holds also for the other components of the angular momentum L_x and L_y.

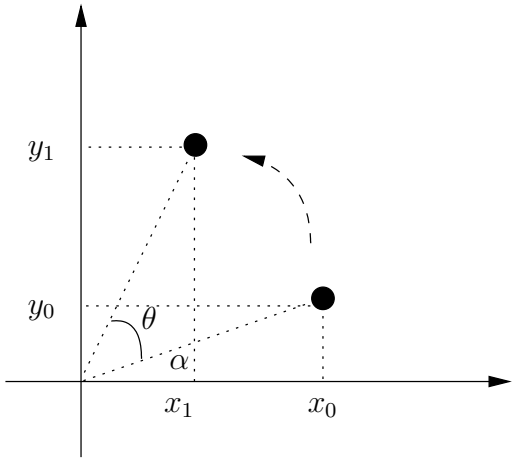
Finally let us notice that also the set of all rotations forms a group. We will discuss the precise nature of this group later in this and the next sections.

8.2.1 Examples and exercises.

Consider for instance the operator

$$O(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{8.10}$$

acting on the space $\mathbf{C}^3$. It represents a rotation of an angle θ around the z-axis. For instance, consider a point whose coordinates are $x_0 = r\cos\alpha\,,\ y_0 = r\sin\alpha$.



After the rotation the new coordinates are

$$\begin{aligned} x_1 &= r\cos(\alpha+\theta) = r\cos\alpha\cos\theta - r\sin\alpha\sin\theta = x_0\cos\theta - y_0\sin\theta\ , \\ y_1 &= r\sin(\alpha+\theta) = r\cos\alpha\sin\theta + r\sin\alpha\cos\theta = x_0\sin\theta + y_0\cos\theta\ . \end{aligned}$$

Exercises.

- Consider the operator L^2

$$L^2 \equiv L_x^2 + L_y^2 + L_z^2 = \sum_{i=1}^{3} L_i^2\ . \tag{8.11}$$

Show explicitly that it commutes with all the components of the angular momentum

$$[L^2, L_x] = 0\ , \quad [L^2, L_y] = 0\ , \quad [L^2, L_z] = 0\ . \tag{8.12}$$

- Check explicitly that

$$(L_x+\mathrm{i}L_y)(L_x-\mathrm{i}L_y) = L^2-L_z^2+\hbar L_z \ , \quad (L_x-\mathrm{i}L_y)(L_x+\mathrm{i}L_y) = L^2-L_z^2-\hbar L_z \ . \tag{8.13}$$

8.3 The angular momentum.

It is clearly important to find the basis of the angular momentum eigenvectors: this can be useful when we want to perform explictly a rotation (in this basis the operator in the exponent becomes just a number) or when the Hamiltonian commutes with L_i (as in the problem of the Hydrogen atom). Of course we can not find simultaneous eignvectors for all components of the angular momentum, since they do not commute, see (8.6). The best we can achieve is to choos one component (for instance L_z) and look for the simultaneous eigenvectors of L^2 and L_z. This is possible thanks to Eq. (8.12). We already know one set of eigenvectors: from (8.9) it follows that any wavefunction $\psi(r^2)$ is an eigenvector with eigenvalue zero for both L^2 and L_z. We can attack the general problem by following an approach similar to the one used to find the energy eigenvectors of the harmonic oscillator hamiltonian.

In this derivation we will be using only two facts:

- the Hermitean properties $L_i^\dagger = L_i$,
- the commutation relations between L_i, given in (8.7), and their consquences.

Thus the results we will derive do not depend on the explicit form of the angular momentum operators (8.6) and hold for any triplet of Hermitean operators satisfying (8.7). In order to stress that the results are general we will use J_x, J_y and J_z to indicate three generic Hermitean operators satisfying (8.6).

Step 1. Suppose that we have an eigenvector of J^2 and J_z

$$J^2|j,m\rangle = \hbar^2 j(j+1)|j,m\rangle \ , \quad J_z|j,m\rangle = \hbar m|j,m\rangle \ , \tag{8.14}$$

where for later convenience we denoted the eigenvalue of J^2 with $\hbar^2 j(j+1)$. Let us show that the possible eigenvalues of J^2 are non-negative (so that we can write them as the $\hbar\sqrt{j(j+1)}$ with $j \geq 0$). This is easily done:

$$\hbar^2 j(j+1) = \langle j,m|J^2|j,m\rangle = ||J|j,m\rangle||^2 \geq 0 \ . \tag{8.15}$$

Step 2. Let us introduce the operators $L_\pm$:

$$J_+ = J_x + \mathrm{i}J_y \ , \quad J_- = J_x - \mathrm{i}J_y \ . \tag{8.16}$$

It is straightforward to check that

$$[J_z, J_+] = \hbar J_+ \ , \quad [J_z, J_-] = -\hbar J_- \ , \tag{8.17}$$

while from (8.12) it is clear that also $J_\pm$ commute with J^2. Now, starting from $|j,m\rangle$, we can generate new eigenvectors by acting with $J_\pm$. By using (8.17) we have

$$J^2 J_\pm |j,m\rangle = \hbar^2 j(j+1) J_\pm |j,m\rangle \ , \quad J_z J_\pm |j,m\rangle = \hbar(m\pm 1) J_\pm |j,m\rangle \ . \tag{8.18}$$

So the state $J_\pm|j,m\rangle$ is an eigenvector of J^2 with the same eigenvalue as $|j,m\rangle$ and is also an eigenvector of J_z with eigenvalue $\hbar(m\pm 1)$. This proves that we can increase or dercrease the quantum number m by an integer.

Step 3. The value of m must be bigger than $-j$ and smaller than j:

$$-j \le m \le j \ . \tag{8.19}$$

This is done by using again that the scalar product is non-degenerate together with (8.13)

$$||J_+|j,m\rangle||^2 = \langle j,m|J_- J_+|j,m\rangle = \langle j,m|(J^2 - J_z^2 - \hbar J_z)|j,m\rangle = \hbar^2\Big(j(j+1) - m(m+1)\Big) \ . \tag{8.20}$$

Since $||J_+|j,m\rangle||^2 \ge 0$ then we must have

$$j(j+1) - m(m+1) = (j-m)(j+m+1) \ge 0 \ , \tag{8.21}$$

which imples $-j-1 \le m \le j$. In the same fashion we can calculate the norm square of $J_-|j,m\rangle$

$$||J_-|j,m\rangle||^2 = \langle j,m|J_- J_+|j,m\rangle = \langle j,m|(J^2 - J_z^2 + \hbar J_z)|j,m\rangle = \hbar^2\Big(j(j+1) - m(m-1)\Big) \ . \tag{8.22}$$

and we find that it is non-negative only if

$$j(j+1) - m(m-1) = (j-m+1)(j+m) \ge 0 \ , \tag{8.23}$$

which imples $-j \le m \le j+1$. By combining these two results we find (8.19).

Step 4. The quantum number j must be either integer of half-integer. From step 2 above, we know that $J_\pm$ act as raising/lowering operators for the J_z quantum number. If we begin with an eigenvector $|j,m\rangle$ we can apply J_+ (or J_-) in order to increase (or decrease) the value of m. On the other hand we cannot violate the bound found above (8.19), thus at a certain point we must find

$$J_+|j,m\rangle = 0 \quad \text{and} \quad J_-|j,-m\rangle = 0 \ . \tag{8.24}$$

This is possible only if $m = j$ (see (8.20)). Now I can start from the ket $|j,j\rangle$ and apply J_- k times to lower the value of the J_z eigenvalue to $m = j-k$. On the other hand we know that $m \ge -j$, which implies that after $k = 2j$ lowering operators have been applied to $|j,j\rangle$ we obtain a vector proportional to $|j,-j\rangle$ and a further J_- would simply lead to

the zero vector. Since k is integer (it counts the number of J_-), then j must be integer of half-integer, as claimed above.

As a final remark, let us specialize this analysis to the angular momentum: in this case (8.6) implies that only *integer* values of j are possible (see the discussion below in the Example section).

8.3.1 Examples and exercises.

Let us focus on the case of the angular momentum and derive some explicit expression for the eigenstates. We already know that any wavefunction $\psi(r^2)$ is an eigenstate with $j = m = 0$. Thus if we find other eigenfunctions (with non-zero eigenvalues) we are free to multiple them by any function of r^2 only without changing the eigenvalues. You already saw this pattern in the study of the Hydrogen atom, where the energy eigenfunctions are the product of a radial function times a purely angular function that is an eigenvector of L^2 and L_z (the spherical harmonics for the 2-sphere). We can derive the explicit form of the spherical harmonics by using the results of this section. We start by checking that the function

$$Y_j^{m=j} = \mathcal{N}_j^j \left(\frac{x + \mathrm{i}y}{r}\right)^j = \mathcal{N}_j^j (\sin\theta)^j \mathrm{e}^{2\pi \mathrm{i} j \phi} \tag{8.25}$$

is an eigenfunction of L^2 and L_z with eigenvalues j and $m = j$. The last relation on thee right hand side is just the rewriting of the Y_j^j in polar coordinates. The quantum number j here can take only integer values, otherwise the function $Y_j^{m=j}$ is not single valued (as it is clear if we look at the form written in polar coordinates and recall that $\phi = 0$ and $\phi = 2\pi$ represent the same point). Let us look at the first non-trivial case $j = 1$. By using the L_- operator we can find the other spherical harmonics

$$Y_1^{m=0} = \frac{L_-}{\hbar\sqrt{2}} \left(\mathcal{N}_1^1 \, Y_1^1\right) = -\mathcal{N}_1^1 \frac{\sqrt{2} z}{r} \ . \tag{8.26}$$

The numerical factor of $\sqrt{2}\hbar$ ensures that the new spherical harmonics is normalized to one if the old one is normalized to one. It follows from (8.22) which in general requires to devide by $\hbar\sqrt{(j-m+1)(j+m)}$ everytime L_- acts on $|j, m\rangle$ if we want to work with vector of norm one.

$$Y_1^{m=-1} = \frac{L_-}{\hbar\sqrt{2}} \left(-\mathcal{N}_1^1 \frac{\sqrt{2} z}{r}\right) = -\mathcal{N}_1^1 \frac{x - \mathrm{i}y}{r} \ . \tag{8.27}$$

You can rewrite these last two equation in polar coordinates and find the expression for the spherical harmonics that you did see in the analysis of the Hydrogen atom. You can repeat the same steps starting from (8.25) with $j = 2$ and find the explicit form of the 5 harmonics of the level 2.

Exercises.

- Calculate $\mathcal{N}_1^1$ in (8.25) by requiring that $\int \bar{Y}_1^1 Y_1^1 d\Omega = 1$

* Consider the wavefunction $\psi = x^2/r^2$. What is the probability of finding the values j and m in a simultaneous measurement of L^2 and L_z?

9 The spin.

We saw that a triplet of operators satisfying the commutation relations (8.7) can admit eigenvectors with a half-integer quantum number j. We also know that this kind of eigenvectors do not appear when we focus on the case of the angular momentum, where the generator take the particular form of Eq (8.6). One might wonder whether the case of half-integer j appears in some interesting physical system or not. The surprising answer is that this case is indeed very common!

9.1 $SO(3)$ representations.

Consider the three wavefunctions (8.25), (8.26) and (8.27) derived in the previous example. They form a basis for the subspace of wavefunctions with $j = 1$ (so the J^2 eigenvalue is $2\hbar^2$ for all these states). We can represent these three states as follows

$$Y_1^1 \leftrightarrow |1,1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \quad , \quad Y_1^0 \leftrightarrow |1,0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \quad , \quad Y_1^{-1} \leftrightarrow |1,-1\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \ . \tag{9.28}$$

From the results summarized in the previous example, we know how L_z and $L\pm$ act that in this subspace

$$\begin{aligned} L_z &= \hbar\Big(|1,1\rangle\langle 1,1| - |1,-1\rangle\langle 1,-1|\Big) \ , \\ L_+ &= \sqrt{2}\hbar\Big(|1,1\rangle\langle 1,0| + |1,0\rangle\langle 1,-1|\Big) \ , \\ L_- &= \sqrt{2}\hbar\Big(|1,0\rangle\langle 1,1| + |1,-1\rangle\langle 1,0|\Big) \ . \end{aligned} \tag{9.29}$$

These operators cen ba written in terms of matrices acting on the vector (9.28)

$$L_z = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \ , \ L_+ = \hbar \begin{pmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{pmatrix} \ , \ L_- = \hbar \begin{pmatrix} 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 \end{pmatrix} \ , \tag{9.30}$$

The three states in (9.28) form the so-called vector representation of the $SO(3)$ rotation group. Let us check that there is a direct relation between the matrices (9.30) and the generators of the rotations as seen in (8.10). In order to see this let us introduce the matrix

$$A = \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & \frac{-1}{\sqrt{2}} \\ \frac{-\mathrm{i}}{\sqrt{2}} & 0 & \frac{-\mathrm{i}}{\sqrt{2}} \\ 0 & 1 & 0 \end{pmatrix} .$$

From eqs. (8.25), (8.26) and (8.27), we can see that A implements a change of basis from the eigenvectors Y_1^1 to the standard cartesian basis where the first eigenfunction is proportional to x and the remaining ones to y and z. In this basis the generators of the rotation around z (L_z) takes a different form with the respect of (9.30)

$$L_z = A\hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} A^{-1} = \hbar \begin{pmatrix} 0 & \mathrm{i} & 0 \\ -\mathrm{i} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} . \tag{9.31}$$

Similar relations hold for L_x and L_y showing that, in this basis, they form the standard generators for the $SO(3)$ rotation group (see the example 8.2.1).

Exercises.

[Op.] One can follow a similar derivation also for the 5 eigenfunctions with $j = 2$. Show that there is a one-to-one correspondence between these eigenfunctions and the symmetric square matrices.

9.2 Spin $1/2$ and $SU(2)$ representations.

So far we have described particles through their position and momentum. Mathematically these observables are related to two Hermitean operators $\hat{x}$ and $\hat{p}$ satisfying the canonical commutation relations (5.4). Since, by hypothesis we are dealing with point-like object, apparently there is no room for any other basic observable and one might think that all other observables should be build by using $\hat{x}$ and $\hat{p}$. (For instance, the angular momentum is given by (8.6), the Hamiltonian is give, in the free case, by Eq. (5.3)). However this is not what happens in nature. On the contrary all known "matter" particles (such as the electron, the muon, the quarks, the neutrinos) are not completly determined by specifying their position[14]. It turns out that matter particles possess additional degrees of freedom called "spin". To be precise this means, for this particles we have the following properties:

[14] Of course in quantum mechanics specifying the position of the particle means that give a wavefunction $\psi(x) = \langle x|\psi\rangle$.

- The spin degrees of freedom are described by a triplet of operators S_x, S_y and S_z satisfying the relations (8.7). A complete set of commuting operators (CSCO) is given, for instance, by $\hat{x}$, S_z and S^2.

- The Hilbert space describing the state of the particle is the tensor product of the Hilbert space $\mathcal{H}_x$ where $\hat{x}$ and $\hat{p}$ act and the Hilbert space $\mathcal{H}_S$ where the S_i act.

- Elementary matter particles with half-integer spin behave as fermions, while those with integer spin behave as boson (and, as we have seen in the previous section this affects the description of multiparticle systems!). For instance, for a spin 1/2 particle the only (eigen)value of S^2 is $3\hbar^2/4$ corresponding to an eigenvalues $s = 1/2$. This implies that $\mathcal{H}_S$ is two dimensional and a basis for this space is given by

$$|s = \frac{1}{2}, m = \frac{1}{2}\rangle \quad , \quad \text{and} \qquad |s = \frac{1}{2}, m = -\frac{1}{2}\rangle \ ,$$

  where as in the previous section, the first and the second number indicate the eigenvalues of S^2 and S_z respectively.

9.2.1 Examples and exercises.

An explicit realization of $\mathcal{H}_S$ is $\mathbf{C}^2$. As usual in the case of finite dimensional spaces, we can realize any operator as a matrix. Conventionally the following choice is taken for the spin operators: $S_a = \frac{\hbar}{2}\sigma_a$, with $a = 1, 2, 3$ and

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \ , \quad \sigma_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} \ , \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \ . \tag{9.32}$$

These σ's are called *Pauli matrices*. In this representation we have

$$|\frac{1}{2}, \frac{1}{2}\rangle \leftrightarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad , \quad \text{and} \qquad |\frac{1}{2}, -\frac{1}{2}\rangle \leftrightarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix} \ . \tag{9.33}$$

These two states are commonly indicated as "spin up" and "spin down" states.

Exercises.

- Check the following property of Pauli matrices

$$[\sigma_a, \sigma_b] = 2\mathrm{i}\epsilon_{abc}\sigma_c \quad , \qquad \sigma_a\sigma_b + \sigma_b\sigma_a = 2\delta_{ab} \ , \tag{9.34}$$

- Show that

$$\mathrm{e}^{\mathrm{i}\phi\sigma_2} = \begin{pmatrix} \cos\phi & \sin\phi \\ -\sin\phi & \cos\phi \end{pmatrix} \tag{9.35}$$

9.3 Addition of two spins.

Consider now a two particle systems whose constituents have spin $s^{(1)}$ and $s^{(2)}$ respectively. As we know, the Hilbert space describing the whole system is the tensor product of the spaces describing the single constituents. In particular, we also need to consider the tensor product of the spaces describing the spin: $\mathcal{H}_{S_1}$ for the first particle and $\mathcal{H}_{S_2}$ for the second one. The total spin of the system is of course $\vec{S} = \vec{S}_1 + \vec{S}_2$, where $\vec{S}_1$ acts only on the first space $\mathcal{H}_1$ and $\vec{S}_2$ on the second one. Then also the components of $\vec{S}$ satisfy the commutation relations (8.6) and so we we should be able to write the states of the total system in terms of the eigenvectors derived in the previous section. The question we want to address now is what are the eigenvalue for the total spin S^2, if we know the eigenvalue of each of the constituents. We have the following result:

> If s_1 and s_2 indicate the spin quantum number of the constituents (that is S_1^2 eigenvalue is $\hbar^2 s_1(s_1+1)$ and similarly for S_2^2), then the possible eigenvalues for the total spin S^2 are s with $|s_1 - s_2| \leq s \leq s_1 + s_2$ and each eigenvalue appears just as one multiplet (a set of $2s+1$ values of S_z).

Let us work out explicitly the simple case of two objects having each one spin 1/2. For instance consider an hydrogen atom: both the proton and the electron have spin 1/2 and we would like to know the spin of the whole atom. The spin states

$$
\begin{aligned}
|\uparrow,\uparrow\rangle &= \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad , \quad |\uparrow,\downarrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} \ , \\
|\downarrow,\uparrow\rangle &= \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad , \quad |\downarrow,\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} \ ,
\end{aligned}
\tag{9.36}
$$

where the first (second) entry refers to the the first (second) particle and we used $\uparrow$ in order to indicate a state with the positive eigenvalue of S_z. Clearly the z-component of the total spin of the state $|\uparrow,\uparrow\rangle$ is $\hbar$ and thus it must represent the eigenvector $|1,1\rangle$. From this vector we can generate the other two states of the triplet with $s=1$

$$
|1,0\rangle = \frac{1}{\sqrt{2}}\Big(|\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle\Big) \ , \quad |1,-1\rangle = |\downarrow,\downarrow\rangle \ . \tag{9.37}
$$

Finally the state $|0,0\rangle$ must be the state with one spin up and one spin down that is orthogonal to $|1,0\rangle$ (since they have a different eigenvalue).

$$
|0,0\rangle = \frac{1}{\sqrt{2}}\Big(|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle\Big) \ . \tag{9.38}
$$

This steps can be repeated in the case of general spins and yield to the result summarized above.

9.3.1 Examples and exercises.

Exercises.

- Consider a composite system with two particle of spin s_1 and s_2 respectively. What is the dimension of the Hilbert space describing the spin degrees of freedom?
- Both the proton and the electron have spin 1/2. Is the hydrogen atom a boson or a fermion ?

Legenda:

$\equiv$	"equivalent by definition"	$\mathbf{C}$	the set of complex numbers
$\exists$	"exists at least one"	$\mathbf{N}$	the set of positive integer numbers
$\exists!$	"exists just one"	$\mathbf{R}$	the set of real numbers
$\forall$	"for all"	$\mathbf{Z}$	the set of integer numbers
$\in$	"belongs to"	$\subseteq$	is contained in