Quantum Mechanics

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Chapter 1

Introduction

These notes are intended to students in the 4th course of the Bachelor in Physics in the University of Granada. So, despite being somewhat self-contained, I assume elementary knowledge from previous courses (e.g. linear algebra, elementary probability, one-dimensional problems in quantum physics, relation between position and momentum, composition of angular momentua, etc.).

Following Steven Weinberg, I make special emphasis on the whys. For example, based on symmetry theory, I discuss why the usual observables (momentum, angular momentum, etc.) commute and act on wave-functions as assumed in quantum physics.

I also provide a substantial number of examples that both help understanding the theoretical concepts as well as connect with active fields of research, such as supersymmetry, renormalization or dualities, among others.

I base mostly on books and notes by Steven Weinberg, David Tong and Robert Griffiths, with a significant amount of my own work. I use Dirac's notation throughout. Also, I try to **boldface** those concepts which are absolutely crucial.

Disclaimer: These notes are in embryonic form, so most likely there're tons of typos.

Chapter 2

Fundamentals of Quantum Mechanics

2.1 Postulates

The modern formulation of Quantum Mechanics (QM) rests on a few postulates. They can be roughly stated as follows.

1. The state of a physics system is described by a normalised vector $|\psi\rangle$ on a (complex) Hilbert space $\mathcal{H}$. Two vectors that differ by a phase represent the same state.

2. Observables $\mathcal{A}$ are represented by Hermitian operators A on $\mathcal{H}$. The possible values of an observable $\mathcal{A}$ are the eigenvalues of A.

3. If the state of a system is described by $|\psi\rangle$, then the probability of obtaining an eigenvalue a in a measurement of $\mathcal{A}$ is $p_a = |\langle\psi|P_a|\psi\rangle|^2$, where P_a is the projector onto the subspace of eigenvectors of A with eigenvalue a, and $\langle|\rangle$ stands for the inner product. (If a is non-degenerated, then the project reads $P_a = |a\rangle\langle a|$ and therefore $p_a = \langle\psi|a\rangle\langle a|\psi\rangle = |\langle\psi|a\rangle|^2$.)

4. If the value of $\mathcal{A}$ is observed to be a, the state of the system immediately afterwards is described by $P_a|a\rangle$.

5. The evolution of the state of the system in time is given by the Schrödinger equation $i\hbar\frac{d|\psi\rangle}{dt} = H|\psi\rangle$ where H is the Hamiltonian operator.

So far I've scrupulously made the difference between the state of a physical system and $|\psi\rangle$, likewise for an observable and A. I don't have any good definition of the former. I rather rely on your previous knowledge and intuitions. Hereafter I also abuse notation and simply use $|\psi\rangle$ for the state, and A for the observable.

There is a number of mathematical concepts (Hilbert space, linear operator, projection, ...) that we must understand to comprehend what these postulate really mean.

2.1.1 Linear algebra

A **Hilbert space** $\mathcal{H}$ is, first and foremost, a vector space, so that any linear combination $\alpha|\psi\rangle + \alpha'|\psi'\rangle \in \mathcal{H}$ for any two vectors $|\psi\rangle, |\psi'\rangle \in \mathcal{H}$ and any two (complex) numbers [1]

[1] There's quite some amazing research about why Hilbert spaces in QM must be complex. We won't dig into it, though.

$\alpha, \alpha' \in \mathbb{C}$. It comes also with an inner (or scalar) product, also known as *bra-ket*, namely a binary operation between two vectors, $\langle\psi|\psi'\rangle \in \mathbb{C}$ that fulfills the following conditions:

1. Antisymmetry: $\langle\psi|\psi'\rangle = \langle\psi'|\psi\rangle^*$.
2. Linearity: $\langle\psi|\alpha'\psi' + \alpha''\psi''\rangle = \alpha'\langle\psi|\psi'\rangle + \alpha''\langle\psi|\psi''\rangle$.
3. Positivity: $\langle\psi|\psi\rangle \geq 0$ with the inequality being saturated only for $|\psi\rangle = 0$.

(Obviously, positivity implies that $\langle\psi|\psi\rangle$ is real.) It follows that the inner product is anti-linear (namely numbers get complex-conjugated) in the first variable. We say that two vectors are orthogonal iff $\langle\psi'|\psi\rangle = 0$.

The scalar product fulfills the Schartz inequality,

$$\langle\psi'|\psi'\rangle\langle\psi|\psi\rangle \geq |\langle\psi'|\psi\rangle|^2 . \tag{2.1}$$

To prove this, let's define

$$|\psi''\rangle \equiv |\psi\rangle - |\psi\rangle' \frac{\langle\psi'|\psi\rangle}{\langle\psi'|\psi'\rangle} . \tag{2.2}$$

(Note that the denominator is zero iff $|\psi\rangle'$ is the zero vector, in which case the Schwartz inequality obviously holds.) Now,

$$\begin{aligned} 0 \leq \langle\psi''|\psi''\rangle\langle\psi'|\psi'\rangle &= \langle\psi|\psi\rangle\langle\psi'|\psi'\rangle - 2\langle\psi|\psi'\rangle\langle\psi'|\psi\rangle + |\langle\psi'|\psi\rangle|^2 \\ &= \langle\psi|\psi\rangle\langle\psi'|\psi'\rangle - |\langle\psi'|\psi\rangle|^2. \end{aligned} \tag{2.3}$$

The scalar product gives rise to a norm, $|||\psi\rangle|| = \sqrt{\langle\psi|\psi\rangle}$. This measures the "size" of vectors and can be used to discuss metric and topology issues such as limits of sequences. Certain very technical points come into play when $\mathcal{H}$ is an inifite-dimensional vector space, such as separability, completeness, etc [2]. I'll deliberately ignore them, since they're irrelevant for our purposes.

What matters for us is that for a given $\mathcal{H}$ there always exists a basis, $\mathcal{B} = \{|\psi_n\rangle\}_{n\in I}$ (I'll avoid specifying the range of n from now on) such that any vector $|\psi\rangle$ can be written as a (potentially infinite) linear combination of elements of the basis; $|\psi\rangle = \sum_n c_n|\psi_n\rangle$, with $c_n = \langle\psi_n|\psi\rangle$.

A very important concept is that of **subspace** of a Hilbert space $\mathcal{H}$. This is a subset $\mathcal{H}' \subset \mathcal{H}$ that is closed under linear combinations. Given a subspace $\mathcal{H}'$, we define the orthogonal complement of $\mathcal{H}'$ as $\mathcal{H}'^{\perp} = \{|\psi\rangle \in \mathcal{H} / \langle\psi'|\psi\rangle = 0 \ \forall|\psi'\rangle \in \mathcal{H}'\}$. Any vector $|\psi\rangle$ can be written in an unique way as $|\psi\rangle = |\psi'\rangle + |\psi'^{\perp}\rangle$, with $|\psi'\rangle \in \mathcal{H}'$ and $|\psi'^{\perp}\rangle \in \mathcal{H}'^{\perp}$. We say that $\mathcal{H}$ is the direct sum of $\mathcal{H}'$ and its orthogonal complement, $\mathcal{H} = \mathcal{H}' \oplus \mathcal{H}'^{\perp}$. A graphical representations of all these concepts is given in Fig. 2.1.

A **complete set of compatible observables (CSCO)** is a set $\{A_i\}$ of mutually compatible observables (i.e. $[A_i, A_j] = 0$) that admits a unique common basis. So, their simulteneous eigenvalues uniquely specify an element of the basis.

[2] To be a Hilbert space, $\mathcal{H}$ must be complete with respect to this norm. Namely, any Cauchy sequence, that is any $\{|\psi_n\rangle\}_{n\in I\subset\mathbb{N}}$ fulfilling that for any $\epsilon > 0$ there exist N such that $|||\psi_n\rangle - |\psi_m\rangle|| < \epsilon$ for all $n, m > N$, must be convergent, namely there must exist $\psi \in \mathcal{H}$ fulfilling that for any $\epsilon > 0$ there exists N for which $|||\psi\rangle - |\psi_n\rangle|| < \epsilon$ for all $n > N$. In other words, any sequence in which consecutive elements get closer and closer, has a limit within the Hilbert space. For the matter of example, $\mathbb{Q}$ with the usual norm given by the absolute value of numbers is not complete; the sequence of rational numbers $\{(1+1/n)^n\}_{n\in\mathbb{N}}$ converges to the Euler's number e, which is irrational. Any non-complete space can be completed by adding all those "holes" left by non-convergent Cauchy sequences. For example, completing $\mathbb{Q}$ gives rise to $\mathbb{R}$.

Figure 2.1: *To be done.*

Linear operators

Linear **operators** on a Hilbert space $\mathcal{H}$ are applications $A : \mathcal{H} \to \mathcal{H}$ that respect the vector structure of the space, namely $A(\alpha|\psi\rangle + \alpha'|\psi'\rangle) = \alpha A|\psi\rangle + \alpha' A|\psi'\rangle$. There are two special operators, the identity, $\mathbb{I}|\psi\rangle = |\psi\rangle$, and the null operator, $0|\psi\rangle = 0$.

Linear operators can be trivially added and multiplied; $(A + B)|\psi\rangle = A|\psi\rangle + B|\psi\rangle$, $(AB)|\psi\rangle = A(B|\psi\rangle)$. In general operators do not commute, namely $AB \neq BA$, or equivalently the **commutator** $[A, B] = AB - BA$ does not vanish. This concept is probably the most important one in QM, so we'll delve into that at length later on.

Within Dirac's notation, we write $\langle\psi|A|\psi'\rangle$, where A, unless otherwise stated, acts on the ket. This'll anyways be of little use, so most important operators in QM are what we call Hermitian.

Given an operator A, we can define the **Hermitian** $A^\dagger$ as the operator satisfying $\langle\psi|A|\psi'\rangle = \langle\psi'|A^\dagger|\psi\rangle^*$. One can trivially show that $(A^\dagger)^\dagger = A$, $(A + B)^\dagger = A^\dagger + B^\dagger$ and $(AB)^\dagger = B^\dagger A^\dagger$. An operator is self-Hermitian [3] (or simply Hermitian) if $A = A^\dagger$. In that case, we write $\langle\psi|A|\psi'\rangle$ irrespective of whether A acts on the ket or on the bra. Two hermitian operators that commute are called compatible. Observables are always represented by Hermitian operators; however there're other important ones, mostly representing symmetries, which aren't necessarily so.

Given a basis $\mathcal{B} = \{|\psi_n\rangle\}$, we can associate a matrix to any linear operator following $A \leftrightarrow (A)_{mn} = \langle\psi_m|A|\psi_n\rangle$. Within this representation, addition and multiplication of operators amounts to addition and multiplication of matrices, while the Hermitian is given by the complex-conjugated matrix. The trace of an operator can be defined as the trace of the corresponding matrix (care in infinite dimension). Hence:

$$\mathrm{tr}(A) = \sum_n \langle\psi_n|A|\psi_n\rangle \,. \tag{2.4}$$

Two more very important concepts are those of eigenvector and eigenvalue. $|a\rangle$ is an **eigenvector** of A with **eigenvalue** a iff $A|a\rangle = a|a\rangle$. It can be shown that, if A is hermitian, then all its eigenvalues are real. Indeed:

$$a\langle a|a\rangle = \langle a|a\mathbb{I}|a\rangle = \langle a|A|a\rangle = a^*\langle a|a\rangle \,. \tag{2.5}$$

(I'll avoid writing explicitly the identity operator hereafter.) So, if $|a\rangle \neq 0$ (which obviously has eigenvalue zero and then is real), then $a = a^*$. Likewise, two eigenvectors of the same operator with different eigenvalues are necessarily orthogonal. Indeed:

$$a\langle a'|a\rangle = \langle a'|Aa\rangle = a'\langle a'|a\rangle \,, \tag{2.6}$$

so if $a \neq a'$ then $\langle a'|a\rangle = 0$.

A very special property of any Hermitian operator A (in finite dimension d) is that there is always a basis built upon eigenvectors of A. Equivalently, there is always a basis in which the corresponding matrix A is diagonal. To show this, let us first note that clearly there is always at least one eigenvector $|a\rangle$ of A with eigenvalue a, because this

[3] In infinite-dimensional Hilbert spaces, there is one further distinction between adjoint and Hermitian operators. As before, we'll deliberately ignore this issue.

Figure 2.2: *To be done.*

is equivalent to saying that the polynomial $\det(A - a\mathbb{I})$ has at least one root, which is guaranteed by the fundamental theorem of algebra. So, $A|a\rangle = a|a\rangle$.

Let us now consider the orthogonal complement of the space spanned by $|a\rangle$, namely $\mathcal{H}_a^\perp = \{|\psi\rangle \in \mathcal{H} / \langle a|\psi\rangle = 0\}$. This subspace is **invariant** under the action of A, namely $A|\psi\rangle \in \mathcal{H}_a^\perp$ for any $|\psi\rangle \in \mathcal{H}_a^\perp$. This works precisely because A is Hermitian. Indeed, $\langle a|A|\psi\rangle = a\langle a|\psi\rangle = 0$, and hence $A|\psi\rangle$ is in $\mathcal{H}_a^\perp$. Therefore, the action of A can be restricted to this subspace, where it becomes a $(d-1)$-dimensional Hermitian matrix, that, again following the reasoning above, admits at least one eigenvector. Precisely because this eigenvector lives in $\mathcal{H}_a^\perp$, is orthogonal to $|\psi\rangle$. Iterating this way, one can obtain a basis of orthogonal eigenvectors of A. This process is shown pictorially in Fig. 2.2. This also implies that the identity operator can be written as

$$\mathbb{I} = \sum_n |a_n\rangle\langle a_n| \,,$$

with the sum running over eigenvalues of a Hermitian A.

Precisely because the eigenvectors of Hermitian operators form a basis, we can write $|\psi\rangle = \sum_n c_n |a_n\rangle$. Hence, given an observable A, and a function $f : \mathbb{R} \to \mathbb{R}$, we can define $f(A)$ simply by requiring that, on an eigenvector $|a\rangle$, $f(A)|a\rangle = f(a)|a\rangle$ and then extending by linearity:

$$f(A) \sum_n c_n |a_n\rangle = \sum_n c_n f(a_n)|a_n\rangle \,.$$

This definition reduces correctly to the case in which f is simply a polynomial, $f(A) = A^k$. For example, $A^2|a\rangle = A(A|a\rangle) = aA|a\rangle = a^2|a\rangle$. In matrix form, this implies that the function of a diagonal matrix is $f(\mathrm{diag}(a_1, a_2, ..., a_n)) = \mathrm{diag}(f(a_1), f(a_2), ..., f(a_n))$.

To see how relevant the hermiticity condition is, let us consider the operator

$$A = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} \,,$$

which is obviously non-Hermitian. The only eigenvectors of A are those multiple of $(1, 0)$, which of course does not expand a basis.

Similarly, two **compatible operators** (or matrices) A and B, $[A, B] = 0$, can be simultaneously diagonalised. Let us simply take the subspace $\mathcal{H}_a = \{|a\rangle \in \mathcal{H}\}$ of eigenvectors of A with eigenvalue a (this does not need to be unidimensional; note also that I from now on avoid indicating the eigenvalue condition since the notation is clear). Again, $\mathcal{H}_a$ is invariant under the action of B if both A and B commute. Indeed, $AB|a\rangle = BA|a\rangle = aB|a\rangle$, which shows that the action of B on a leaves a within $\mathcal{H}_a$ ($B|a\rangle$ is still an eigenvector of A with eigenvalue a). Therefore, just as before, we can restrict the action of B to $\mathcal{H}_a$, where we can find an orthogonal basis of eigenvectors of B which, obviously, will be also eigenvectors of A (cause they all have the same eigenvalue a). Iterating this process, we can find a common orthogonal basis of eigenvectors of A and B.

Note however, that there can exist a basis in which A is diagonal while B is not, even if they commute. For example,

$$A = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \,, \quad B = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \,.$$

Also important is that two operators can be non-commuting and still have *some* common eigenvector. For example

$$P = \begin{pmatrix} 1 & i & 0 \\ -i & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad Q = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

do not commute, and still $|\psi\rangle = (0, 0, 1)$ is eigenvector of both. In such case, necessarily, $[P, Q]|\psi\rangle = 0$.

Expectation value

The **expectation** (or expected) value of a random variable is the average value that one'd obtain after several (infinite) outcomes. Hence it is the sum of all outcomes weighted by their probability. For example, the expected profit when betting colour (say red) in a roulette is

$$\frac{18}{37} - \frac{19}{37} = -\frac{1}{37}.$$

Not surprise that this number is negative; casinos always win (potential exception playing black-jack).

According to the third postulate of QM, the probability of obtaining a in a measurement of A is $|\langle a|\psi\rangle|^2$. Therefore, the expectation value of A when the system is in the state $|\psi\rangle$, that we denote as $\langle A\rangle_\psi$, reads:

$$\langle A\rangle_\psi = \sum_n a_n |\langle a_n|\psi\rangle|^2 = \sum_n a_n \langle\psi|a_n\rangle\langle a_n|\psi\rangle = \sum_n \langle\psi|A|a_n\rangle\langle a_n|\psi\rangle = \langle\psi|A|\psi\rangle\,. \tag{2.7}$$

In general, $\langle f(A)\rangle_\psi \neq f(\langle A\rangle_\psi)$. In particular, $\langle A^2\rangle_\psi \geq \langle A\rangle_\psi^2$. The proof is simple:

$$0 \leq \langle (A - \langle A\rangle_\psi)^2\rangle_\psi = \langle A^2 + \langle A\rangle_\psi^2 \mathbb{I} - 2\langle A\rangle_\psi A\rangle_\psi = \langle A^2\rangle_\psi - \langle A\rangle_\psi^2\,. \tag{2.8}$$

Iff $|\psi\rangle$ is an eigenvector of A, then the inequality is saturated. A measure of departure from this situation (a measure of "quantumness") is given precisely by the mean square deviation,

$$\Delta_\psi^2 A \equiv \langle (A - \langle A\rangle_\psi)^2\rangle_\psi\,.$$

The (generalised) Heisenberg uncertainty principle states that

$$\Delta_\psi A \Delta_\psi B \geq \frac{1}{2}|\langle [A, B]\rangle_\psi|\,.$$

To prove this, we first note that $\Delta_\psi^2 A \equiv \langle\psi_A|\psi_A\rangle$, with $|\psi_A\rangle = (A - \langle A\rangle_\psi)|\psi\rangle$. Now we can apply the Schwartz's inequality to $|\psi_A\rangle$ and $|\psi_B\rangle$, $\Delta_\psi^2 A \Delta_\psi^2 B \geq |\langle\psi_A|\psi_B\rangle|^2$, which implies

$$\Delta_\psi A \Delta_\psi B \geq |\langle\psi_A|\psi_B\rangle| \geq |\mathrm{im}\langle\psi_A|\psi_B\rangle|\,.$$

Elaborating on the RHS:

$$\begin{aligned} \langle\psi_A|\psi_B\rangle &= \langle\psi|(A - \langle A\rangle_\psi)(B - \langle B\rangle_\psi)|\psi\rangle \\ &= \langle\psi|AB - A\langle B\rangle_\psi - \langle A\rangle_\psi B + \langle A\rangle_\psi\langle B\rangle_\psi|\psi\rangle \\ &= \langle\psi|AB|\psi\rangle - \langle A\rangle_\psi\langle B\rangle_\psi\,. \end{aligned} \tag{2.9}$$

Now, for Hermitian operators, $\langle\psi|AB|\psi\rangle^* = \langle\psi|BA|\psi\rangle$ and therefore (taking into account that $\mathrm{im}(z) = \frac{1}{2i}(z - z^*)$ for all $z \in \mathbb{C}$),

$$\mathrm{im}\langle\psi_A|\psi_B\rangle = \frac{\langle\psi|[A,B]|\psi\rangle}{2i} = \frac{\langle[A,B]\rangle_\psi}{2i}$$

from where

$$\Delta_\psi A \Delta_\psi B \geq \frac{1}{2}|\langle[A,B]\rangle_\psi|\,.$$

In the particular case of position and momentum, $[X,P] = i\hbar$, we obtain the usual Heisenberg uncertainty principle $\Delta_\psi X \Delta_\psi P \geq \frac{\hbar}{2}$.

Projectors

A very important case of Hermitian operator (and hence observable) is projectors. They appear in the third and fourth postulates of QM. A linear operator P is a **projector** iff $P = P^\dagger$ and $P^2 = P$. It is trivial to show that the only eigenvalues of P are 1 or 0. There is a one-to-one correspondence between an operator P and the subspace $\mathcal{H}_P$ of $\mathcal{H}$ onto which it projects, defined by $\mathcal{H}_P = \{|\psi\rangle \in \mathcal{H}/P|\psi\rangle = |\psi\rangle\}$; namely those eigenvectors with eigenvalue 1. All vectors in $\mathcal{H}_P^\perp$ have eigenvalue 0. All others have no definite eigenvalue.

This makes also very easy to write projectors using Dirac's notation. Let $\{|\psi\rangle_n\}$ be an orthogonal basis of $\mathcal{H}_P$. Then $P = \sum_n |\psi_n\rangle\langle\psi_n|$. The identity is the extreme case of projector.

If two projectors commute, the subspace associated to one is invariant under the action of the other. For example, let us consider

$$P = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}\,, \quad Q = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}\,. \tag{2.10}$$

which fulfill $[Q,P] = 0$. The subspace associated to P is spaned by the vectors $(1,0,0)$ and $(0,1,0)$, while the one of Q is spaned by $(0,1,0)$ and $(0,0,1)$. However, note than none of the subspaces is included in the other, nor are they orthogonal.

The product of projectors is in general not a projector. Indeed,

$$(PQ)^\dagger = Q^\dagger P^\dagger = QP\,,$$

and

$$(PQ)^2 = PQPQ\,.$$

However, if they commute it is clear that the projector conditions hold. The sum of projectors is not a projector, even if they commute. However, the combination $P+Q-PQ$ is a projector if P and Q commute. For example:

$$\begin{aligned}(P+Q-PQ)^2 &= P + PQ + PQ + QP + Q - QPQ - PQP - PQ - PQPQ \\ &= P + Q - PQ\,.\end{aligned} \tag{2.11}$$

In the second equality we have used that they commute.

This discussion helps us understanding why QM is the way it is, and why it is so different from classical mechanics. Within classical mechanics, irrespective of the state

of the system, all propositions about Nature are either true or false; e.g. "The energy of the system between E_0 and E_1". Hence the space of states in classical mechanics is simply a phase space $\mathcal{M}$ (e.g. $\mathcal{M} = \{(x,p) \in \mathbb{R}^2\}$ for the simple harmonic oscillator); propositions being represented by subsets of $\mathcal{M}$ (e.g. $\{(x,p) \in \mathcal{M}/E_0 < x^2 + p^2 < E_1\}$ for the above proposition).

One of the greatest achievement of humankind is Heisenberg's realisation that some propositions are actually neither true nor false (a philosopher could complain that they shouldn't be call propositions then). That's why QM space of states must be something else. With the astonishing discovery that it must be a Hilbert space, it becomes clear that propositions are represented by subspaces of $\mathcal{H}$ or equivalentely by the corresponding projectors. Thus, the proposition P is true when $P = 1$ (namely $|\psi\rangle$ is an eigenvector of P with eigenvalue 1) and false if $P = 0$ ($P|\psi\rangle = 0$). But it's *ill-defined* (so neither true nor false) otherwise.

Following standard logic, propositions can be combined into more complex propositions, e.g. $P \wedge Q$ (read P and Q, which is true iff both P and Q are true), $P \vee Q$ (read P or Q, which is true iff any of them or both is true).

This implies that the core difference between classical and QM is that observables do not commute in general. Classical mechanics is the limit of QM in which only commuting operators survive. If we focus on a physical system where all relevant observables commute, then all our intuitions about classical mechanics hold. But it doesn't otherwise, and that's painful.

The last ingredient to get a fully practical comprehension of the postulates of QM is time evolution. But that's trivial. One only needs to solve Schrödinger equation:

$$|\psi(t)\rangle = \exp\left(-\frac{iHt}{\hbar}\right)|\psi_0\rangle\,. \tag{2.12}$$

We have seen before how to define the function of an operator, in particular the exponential: We must work in the basis of eigenstates of the operator H. Hence, if we have $|\psi_0\rangle = \sum_n c_n |E_n\rangle$, we simply have:

$$|\psi(t)\rangle = \sum_n c_n \exp\left(-\frac{iE_n t}{\hbar}\right)|\psi_n\rangle\,. \tag{2.13}$$

Example 1. Supersymmetric quantum mechanics

A supersymmetric QM system is one in which the Hamiltonian fulfills the supersymmetric algebra $H = \frac{1}{2}\{Q, Q^\dagger\}$ with $Q^2 = 0$. Q is called the supercharge. We will prove that:

(a) Show that $\langle H\rangle_\psi \geq 0$ and therefore that there is no state with negative energy.

(b) Prove that the subspace of eigenvectors of H with energy E is invariant under the action of both Q and $Q^\dagger$.

(c) Within this subspace, define $F = \frac{1}{2E}Q^\dagger Q$. Show that F is Hermitian, commutes with H and has eigenvalues 0 and 1. Argue then that both eigenvalues must be realised and therefore the eigenspace of energy $E \neq 0$ is degenerated.

First, note that Q is a sort of square root of the Hamiltonian. In regard of (a), we simply have:

$$2\langle\psi|H|\psi\rangle = \langle\psi|Q^\dagger Q + QQ^\dagger|\psi\rangle = |Q|\psi\rangle|^2 + |Q^\dagger|\psi\rangle|^2 \geq 0\,. \tag{2.14}$$

For (b), we only need to prove that H commutes with both Q and $Q^\dagger$:

$$2[H,Q] = [QQ^\dagger, Q] + [Q^\dagger Q, Q] = QQ^\dagger Q - QQ^\dagger Q = 0\,, \tag{2.15}$$

having ignored Q^2 and $(Q^\dagger)^2$ terms.

About (c), it is trivial to show that $F = F^\dagger$ and that $[F,H] = 0$. That it has eigenvalues 0 and 1 follows from it being a projector (see next section), namely $F^2 = F$:

$$F^2 = \frac{1}{4E^2}Q^\dagger QQ^\dagger Q = \frac{1}{4E^2}Q^\dagger(2H - Q^\dagger Q)Q = \frac{1}{2E}Q^\dagger Q = F\,. \tag{2.16}$$

Hence, eigenvectors $|f\rangle$ must fulfill $f^2 = f$ and hence $f = 0, 1$. At least one of the eigenvalues must be realised within the subspace of energy E. Say it is $f = 0$. Then, however, $Q^\dagger|0\rangle$ has $f = 1$:

$$\frac{1}{2E}(Q^\dagger Q)Q^\dagger|0\rangle = \frac{1}{2E}(2H - QQ^\dagger)Q^\dagger|0\rangle = Q^\dagger|0\rangle\,. \tag{2.17}$$

Likewise, trivially $Q^\dagger|1\rangle = 0$. Therefore, both eigenvalues are realised and therefore the subspace of energy E is degenerated, provided $E \neq 0$.

2.1.2 Density matrix

It is often the case that we do not know what the state of the system is, but only the probability p_n of the system to be in one or another state $|\psi\rangle_n$. In such case, we describe the "state" of the system with a **density matrix** ρ, defined by

$$\rho = \sum_n p_n|\psi_n\rangle\langle\psi_n|\,, \tag{2.18}$$

with $\sum_n p_n = 1$.

The probabilities arising in the density matrix represent our ignorance about the state of the system. This has nothing to do with the probabilities arising in measurements of observables given a state. This probability is essential, rooted in Nature, is not part of our ignorance about Nature (provided one accepts that there are no hidden variables; more about this later). In one case we have incomplete information, in the other we do not.

The density matrix can be also thought as describing a collection (or **ensemble**) of identical systems, in which a fraction p_n of them are in the state $|\psi_n\rangle$.

We say that a state like ρ is a **mixed** state, while if the state of the system is given by a vector $|\psi\rangle$ we say it is **pure**. Of course, they both coincide when $p_n = 1$ for some n. In that case, $\rho = |\psi_n\rangle\langle\psi_n|$. Describing the state of the system using a vector or using the projector that projects onto the subspace spanned by this vector is completely equivalent.

We can easily check that $\mathrm{tr}(\rho) = 1$. Indeed:

$$\mathrm{tr}(\rho) = \sum_m\sum_n p_n\langle\phi_m|\psi_n\rangle\langle\psi_n|\phi_m\rangle = \sum_m\sum_n p_n\langle\psi_n|\phi_m\rangle\langle\phi_m|\psi_n\rangle = \sum_n p_n = 1\,.$$

Now, because ρ is a Hermitian operator, we can also write it as a sum of projectors onto the corresponding eigenspaces, weighted by the eigenvalues:

$$\rho = \sum_n p'_n |p'_n\rangle\langle p'_n| \,.$$

It turns out that also $\sum_n p'_n = 1$ because the trace is basis invariant. So, two seemingly different descriptions of the same mixed state are equivalent; in one, the probabilities extend to pure states which are not necessarily orthogonal, in the other the ignorance is about which of the different elements of an orthogonal basis is the one the system is.

Certain considerations that hold for pure states can be extended to mixed states. For example, the probability of obtaining a in a measurement of A if the system is in the mixed state ρ is:

$$p_a = \sum_n p'_n |\langle p'_n|a\rangle|^2 = \sum_n p'_n \langle a|p'_n\rangle\langle p'_n|\phi_a\rangle = \langle a|\rho|a\rangle = \langle\rho\rangle_a \,.$$

(If a is degenerated one only needs to sum the expression above over all elements of the subspace associated to a.)

Likewise, the expectation value of A on ρ is defined by

$$\langle A\rangle_\rho = \sum_n p'_n \langle p'_n|A|p'_n\rangle = \sum_n \langle p'_n|Ap'_n|p'_n\rangle = \mathrm{tr}(A\rho) \,.$$

It is also trivial to prove that a state is pure iff $\rho^2 = \rho$. The first implication is easy. If $\rho = |\psi\rangle\langle\psi|$, then

$$\rho^2 = |\psi\rangle\langle\psi|\psi\rangle\langle\psi| = \rho \,.$$

Viceversa is not as trivial but still straightforward. Let's assume that $\rho^2 = \rho$, with $\rho = \sum_i p_i |p_i\rangle\langle p_i|$ written in the orthonormal basis of eigenstates of ρ. Then

$$\rho^2 = \sum_{ij} p_i p_j |p_i\rangle\langle p_i|p_j\rangle\langle p_j| = \sum_i p_i^2 |p_i\rangle\langle p_i| \,, 0 = \rho^2 - \rho = \sum_i (p_i^2 - p_i)|p_i\rangle\langle p_i| \,.$$

If we now take the expectation value of this expresion for the state $|p_j\rangle$, we get:

$$0 = \sum_i (p_i^2 - p_i)\langle p_j|p_i\rangle\langle p_i|p_j\rangle = p_j^2 - p_j \Rightarrow p_j = 1$$

or $p_j = 0$. This implies that ρ is a pure state.

A different way of seeing this is that, if $\rho^2 = \rho$, then ρ is a projector (only eigenvalues 0 and 1), but it has at most a one-dimensional projection space with eigenvalue 1 because $\mathrm{tr}[\rho] = 1$.

A condition equivalent to $\rho^2 = \rho$ is $\mathrm{tr}[\rho^2] = 1$.

2.1.3 Continuous spectrum

In infinite-dimensional Hilbert spaces, operators can have continuous spectrum. Namely, X has an (continuous) infinite number of eigenstates $|x\rangle$ with $x \in \mathbb{R}$. So can say that $\mathcal{B} = \{|x\rangle\}$ expands a basis of $\mathcal{H}$ [4].

[4] Being rigorous, this is not true. Operators like position don't have actual eigenvectors, though there're vectors which fulfill that $||(X - \lambda)|\psi\rangle||$ is as small as we like. The limit of sequences of these vector doesn't belong to $\mathcal{H}$ though, but rather to the space of distributions.

Since different x represent different eigenvectors, we should have some notion of orthogonality: $\langle x|x'\rangle = \delta(x-x')$.

As such, expressions like $|\psi\rangle = \sum_n \langle\psi_n|\psi\rangle|\psi_n\rangle$ become

$$|\psi\rangle = \int dx \langle x|\psi\rangle|x\rangle \equiv \int dx \psi(x)|x\rangle\,.$$

Likewise, we have a spectral decomposition of the identity of the form $\mathbb{I} = \int dx|x\rangle\langle x|$.

Another way of thinking about this is assuming that the space is not really infinite but compact. In such case, x is not real, but can take so many values that we can approximate it by real numbers.

The function $\psi(x)$ is what you should know as **wavefunction**. Seeing this way, is nothing but the coefficients of ψ in the basis of (continuous) eigenstates of certain operator. We'll see how operators act on wavefunction representation when we come to symmetries, but let's make a quick reminder:

$$X\psi(x) = x\psi(x)\,, \tag{2.19}$$
$$P[\psi(x)] = i\hbar\psi'(x)\,; \tag{2.20}$$

the generalization to higher dimensions should be trivial.

The scalar product in terms of wavefunctions becomes:

$$\langle\psi|\phi\rangle = \int dx \psi(x)^*\phi(x)\,.$$

Likewise, unit norm implies that

$$\int dx|\psi(x)|^2 = 1\,,$$

so that $\psi(x)$ is essentially a probability density.

So the **Dirac's delta function** represents itself the wavefunction of $|x\rangle$. Thus, an example of vectors that approach $|x\rangle$ in wavefunction form are:

$$\delta(x-x') = \frac{1}{\epsilon\sqrt{\pi}} e^{\frac{-(x-x')^2}{\epsilon^2}}\,;$$

in the limit $\epsilon \to 0$. Another useful representation of Dirac's delta is

$$\delta(x-x') = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk e^{ik(x-x') - \frac{\epsilon^2 k^2}{4}}\,;$$

again in the limit $\epsilon \to 0$. Usually, we'll simply ignore this latter ϵ.

There're certain subtleties when working with continuous spectrum. A recurrent one is care with commutators and traces. For example:

$$\mathrm{tr}([A,B]) = \mathrm{tr}(AB - BA) = \mathrm{tr}(AB) - \mathrm{tr}(BA) = 0\,. \tag{2.21}$$

However, for position and momentum we have $[X,P] = i\hbar$, which seems contradictory.

The core of the problem here is that the trace is not well defined in infinite dimensions, basically.

Perhaps the most important operator in QM (from certain perspective) is the Hamiltonian. Hamiltonian for systems for particles with space-degrees of freedom (e.g. not spins only) have in general discrete as well as continuous spectrum.

For a single particle, we have:

$$H = \frac{P^2}{2m} + V(X)\,,$$

where V is the potential.

Some things that you should've seen already:

1. For potentials fulfilling that $V(x) \to \infty$ for $|x| \to \infty$; as for example the harmonic oscillator $V(x) = \frac{1}{2}kx^2$. (Yet one more example is the infinite-well potential.) In this case, we find an infinite non-continuous (i.e. discrete) number of eigenstates. These states expand a basis.

2. For potentials fulfilling that $V(x) \to$ constant for $|x| \to \infty$, as for example the finite-well potential or the Dirac's delta potential. In this case, there'll be a finite number of discrete states as well as a continuum.

The spectrum of the aforementioned bound states is non-degenerate. To show why, assume the contrary. Then:

$$-\frac{\hbar^2}{2m}\psi''(x) + V(x)\psi(x) = E\psi(x)\,, \quad -\frac{\hbar^2}{2m}\psi''(x) + V(x)\psi(x) = E\phi(x)\,. \tag{2.22}$$

Take now the so-called Wronskian:

$$W(\psi, \phi) = \psi\phi' - \psi'\phi\,.$$

This is space-independent:

$$W'(x) = \psi(x)\phi''(x) - \psi''(x)\phi(x) = \frac{2m}{\hbar^2}(\psi(x)\,[V(x) - E)\phi(x) - \psi(x)(V(x) - E]\,\phi(x)) = 0\,.$$

For bound (normalisable) states, $\phi(x), \psi(x) \to 0$ for $|x| \to \infty$, and so $W(x) \to 0$ in this limit. So together with the previous condition, $W(x) = 0$ everywhere, implying:

$$\frac{\psi'}{\psi} = \frac{\phi'}{\phi} \Rightarrow \log\psi = \log\phi + C \Rightarrow \psi = \alpha\phi\,.$$

Since both differ by a constant only, they represent the same state. (This argument fails for continuous states, cause they don't go to zero at large $|x|$; and indeed e^{ikx} and e^{-ikx} have the same energy while being different states.)

Example 2. 2-dimensional delta and renormalization

In order to going further than previous courses, let's look at the energy states of the 2d-delta potential:

$$-\frac{\hbar^2}{2m}\nabla^2\psi(x) - g\delta^2(x)\psi(x) = E\psi(x)\,,$$

where now $x \in \mathbb{R}^2$.

Let's do some dimensional analysis: $[\delta^2] = L^{-2}$ (cause one integrates $\int d^2x\delta^2(x)$ to get 1, adimensional); $[\psi] = L^{-1}$ (because $\int dx|\psi(x)|^2 = 1$); $[E] = ML^2T^{-2}$; $[\hbar] = ML^2T^{-1}$ (remember, $\hbar$ is measured in Js). Therefore, $[g] = ML^4T^{-2}$.

Altogether, we have that there's no way to make E depend on g, m, $\hbar$. Easy to prove:

$$\begin{aligned}[m]^a[g]^b[\hbar]^c = ML^2T^{-2} &\Rightarrow (M^a)(M^bL^{4b}T^{-2b})(M^cL^{2c}T^{-c}) = ML^2T^{-2} \\ &\Rightarrow 4b + 2c = 2\,, -2b - c = -2 \end{aligned} \tag{2.23}$$

which are obviously incompatible. This is peculiar of 2d.

Let's anyway proceed with the computation of eigenvalues, first doing some redefinition of parameters, multiplying by $m/\hbar^2$ the previous eq:

$$-\frac{1}{2}\nabla^2\psi(x) - \tilde{g}\delta^2(x)\psi(x) = \tilde{E}\psi(x)\,,$$

with

$$\tilde{g} = \frac{mg}{\hbar^2}\,, \quad \tilde{E} = \frac{mE}{\hbar^2}\,.$$

We'll try to solve using Fourier analysis: instead of solving for ψ, we'll solve for its coefficients $\tilde{\psi}$: $\psi(x) = \frac{1}{2\pi}\int d^2k'\tilde{\psi}(k')e^{ik'x}$. We also use the delta representation given by $\delta^2(x) = \frac{1}{(2\pi)^2}\int d^2k'e^{ik'x}$ (notice the different with respect to the one-dimensional delta, it's simply a factor of 2π more).

We'll substitute ψ by its Fourier expansion in the free part, but take $\psi(x) = \psi(0)$ in the interacting part (after all, that's the only value the δ sees). We obtain:

$$\frac{1}{2\pi}\int d^2k'(\frac{k'^2}{2} - \tilde{E})\tilde{\psi}(k')e^{ik'x} = \frac{\tilde{g}}{(2\pi)^2}\int d^2k'e^{ik'x}\psi(0)\,. \tag{2.24}$$

Let's now multiply both sides by e^{-ikx} and integrate over x:

$$\frac{1}{2\pi}\int d^2x\int d^2k'(\frac{k'^2}{2} - \tilde{E})\tilde{\psi}(k')e^{i(k'-k)x} = \frac{\tilde{g}}{(2\pi)^2}\int d^2x\int d^2k'e^{i(k'-k)x}\psi(0) \tag{2.25}$$

which, simplyfing (notice that $\int d^2xe^{i(k'-k)x} = (2\pi)^2\delta^2(k'-k)$), is:

$$2\pi(\frac{k^2}{2} - \tilde{E})\tilde{\psi}(k) = \tilde{g}\psi(0)\,. \tag{2.26}$$

So, we've completed our task of determining the Fourier coefficients of the bound states:

$$\tilde{\psi}(k) = \frac{\tilde{g}}{2\pi}\frac{\psi(0)}{(k^2/2 - E)}\,. \tag{2.27}$$

In order to fix E, we use the Fourier expression of $\psi(0)$ itself:

$$\psi(0) = \frac{1}{2\pi}\int d^2k\tilde{\psi}(k) = \frac{\tilde{g}}{2\pi}\int d^2k\frac{\psi(0)}{k^2/2 - E}\,. \tag{2.28}$$

The result would be immediate if we knew how to solve the integral. (For example in 1d is trivial.) However, $\int d^2k/k^2$ diverges:

$$\int d^2\vec{k}\frac{1}{\vec{k}^2/2 - E} = 2\pi\int_0^\infty dk\frac{k}{k^2/2 - E} \to \infty\,. \tag{2.29}$$

(I've written explicity the vector notation to make clear that we've made a change of variables to polar coordinates: $d^2\vec{k} = kdkd\theta$.)

OK, so this infinity is probably what is telling us that our previous approach based on dimensional analysis works: there're no bound states.

However, we should keep in mind that, after all, the delta potential is simply an approximation to a more complicated potential of which we don't know well the fine details. On the basis of this ignorance, we should admit that we don't know how things behave at large values of k, say below some threshold $k < \Lambda$. This amount to *regularising* the integral as follows:

$$2\pi \int_0^\infty dk \frac{k}{k^2/2 - E} \to \int_0^\Lambda dk \frac{k}{k^2/2 - E} = 2\pi \log\left(1 - \frac{\Lambda^2}{2E}\right).$$

Λ is known as the *UV cutoff*.

Let's see now how equation Eq. (2.28) looks:

$$1 = \frac{\tilde{g}}{(2\pi)^2} \int d^2k \frac{1}{k^2/2 - E} = \frac{\tilde{g}}{2\pi} \log(1 - \frac{\Lambda^2}{2E}),$$

from where

$$E = -\frac{\Lambda^2}{2} \frac{1}{e^{2\pi/\tilde{g}} - 1}.$$

The only way to make E independent of Λ is assuming that $\tilde{g}$ depends itself on Λ. Essentially, we're saying that our description of the physics changes depending on the scales we explore, and that dependence is captured in $\tilde{g}(\Lambda)$. It must be:

$$\tilde{g}(\Lambda) = \frac{2\pi}{\log(1 - \Lambda^2/(2E))}.$$

The physical interpretation of this is that the effective strength of the potential depends on the energy explored. The potential will be more or less attractive for particles of different incoming energies.

Interestingly, $\tilde{g} \to 0$ for large Λ. We say this system is asymptotically free. Same happens with strong interactions unlike electromagnetic ones (quarks which are closer and closer -large distances amount to short energies- are almost free, but if they're separated they interact strongly, like a spring).

Why didn't we face this problem before, if we never know in detail the shape of the potential are minuscule distances? Well, one thing is that we don't know this, but still can insist on describing the system that way (even if it won't be accurate at small scales); a different thing is not being even allowed to assume this description of the system. This latter thing is what happens in the 2d-delta, and also what occurs essentially in the description of interacting relativistic quantum particles.

Example 3. Duality between Coulomb and harmonic oscillator in 2D

We will now solve the spectrum of the Hydrogen atom in 2D. The Hamiltonian in coordinate space reads:

$$H = -\frac{\hbar}{2m}\nabla^2 - \frac{\alpha}{r}, \quad \nabla^2 = \partial_r^2 + \frac{1}{r}\partial_r + \frac{1}{r^2}\partial_\theta^2. \tag{2.30}$$

We first make the change of variables $r = \rho^2$, $\theta = 2\phi$; from where:

$$\partial_r = \partial_r \rho \partial_\rho + \partial_r \phi \partial_\phi = \frac{1}{2\rho} \partial_\rho \ . \tag{2.31}$$

Hence,

$$\nabla^2 = \frac{1}{2\rho}\partial_\rho \left(\frac{1}{2\rho}\partial_\rho \right) + \frac{1}{\rho^2}\frac{1}{2\rho}\partial_\rho + \frac{1}{4\rho^4}\partial_\phi^2 = \frac{1}{4\rho^2}\left(\partial_\rho^2 + \frac{1}{\rho}\partial_\rho + \partial_\phi^2 \right) \tag{2.32}$$

which is nothing but the Laplacian written in polar coordinates, up to a factor of $1/\rho^2$. Therefore, the eigenvalue equation $H\Psi = E\Psi$ reads:

$$\left(-\frac{\hbar}{8m}\nabla^2 - \alpha \right) \Psi = E\rho^2 \Psi \Leftrightarrow \left(-\frac{\hbar}{8m}\nabla^2 - E\rho^2 \right) \Psi = \alpha \Psi \, . \tag{2.33}$$

If we make the definitions $\mu = 4m$ and $\omega^2 = -E/2m$, we obtain:

$$\left(-\frac{\hbar}{2\mu}\nabla^2 + \frac{1}{2}\mu\omega^2\rho^2 \right) \Psi = \alpha \Psi \, . \tag{2.34}$$

This is simply the 2D harmonic oscillator. We can trivially obtain the spectrum of this latter one on the basis of creation and annihilation operators. Let's see how first in the simplest 1D harmonic oscillator. We can define the annihilation operator

$$a = \sqrt{\frac{\mu\omega}{2\hbar}} X + \frac{i}{\sqrt{2\mu\hbar\omega}} P \, . \tag{2.35}$$

The creation operator is simply the hermitian $a^\dagger$. It can be trivially checked that $[a, a^\dagger] = 1$.

Noticing that

$$a^\dagger a = \frac{1}{2\mu\hbar\omega}P^2 + \frac{\mu\omega}{2\hbar}X^2 - \frac{i}{2\hbar}[X, P] = \frac{1}{\hbar\omega}\left(\frac{1}{2\mu}P^2 + \frac{1}{2}\mu\omega^2 X^2 + \frac{1}{2} \right) \ ; \tag{2.36}$$

we can write the Hamiltonian as follows:

$$H = \hbar\omega(a^\dagger a + \frac{1}{2}) \, . \tag{2.37}$$

It can be trivially proven that $[H, a] = -\hbar\omega a$, and $[H, a^\dagger] = \hbar\omega a^\dagger$. Note also that, if $|E\rangle$ is an eigenstate of H, then $a|E\rangle$ has also well defined energy $E - \hbar\omega$:

$$Ha|E\rangle = [H, a]|E\rangle + aH|E\rangle = (E - \hbar\omega)a|E\rangle \, . \tag{2.38}$$

This Hamiltonian is bounded from below, so the only way to fulfill this is that there is some $|E\rangle$ such that $a|E\rangle = 0$, otherwise there will be infinite states of negative energy resulting from applying a over and over. This state has energy $\hbar\omega$. The rest of eigeneneries are of the states $a^\dagger|0\rangle$ [5].

[5] There cannot be any other energy in between. The reason is that, upon applying a over the coresponding state $|\psi\rangle$, we would get negative energy, unless $a|\psi\rangle = 0$, but this implies $a|\psi\rangle$ has zero energy and we have seen that one-dimensional systems are not degenerated.

For the 2D oscillator, we simply have two oscillators (one in x direction, another in y), therefore:

$$E = \hbar\omega(n_x + n_y + 1)\,. \tag{2.39}$$

Now, back to the correspondence with Hydrogen atom, notice that the role of the energy in the oscillator is played by the Coulomb α. Then:

$$\alpha^2 = \hbar^2\omega^2(N+1)^2 = \hbar^2\frac{-E}{2m}(N+1)^2 \Rightarrow E = -\frac{2m\alpha^2}{(N+1)^2}\,. \tag{2.40}$$

Things we have learnt: 2D Hydrogen atom and 2D harmonic oscillator are dual to each other. The negative energies of the Hydrogen atom result from the positive ones of the Coulomb. Compare with the 3D result: $E \sim -\alpha^2/n^2$. SOmething similar works here, but the math is way heavier.

We have obtained a duality between the 2D Hydrogen atom and the 2D harmonic oscillator. They are one and the same thing, though looked from different perspectives. None of them is fundamental, simply different realisations of underlying reality (which we think is the symmetry).

These two seemingly different descriptions of the same physical situation being equivalent is the simplest realisation of a duality. Dualities are commonplace in physics, and they are active field of investigation. Among the most dramatic examples of dualities, we find the physical equivalence of a system of fermions known as Thirring model and a system of bosons known as Sine-Gordon model; in the first, fermions are fundamental, while bosons appear as bound states of fermions, while in the second bosons are fundamental and fermions appear as certain field configurations known as solitons. But the by-far-most spectacular physics duality comes under the name of AdS/CFT by Juan Maldacena, who established the physical equivalence between quantum theories of gravity in d space-time dimensions and theories with no gravity in $d-1$ dimensions.

2.2 Composite systems

The Hilbert space of the composed system involving two QM systems described by $\mathcal{H}$ and $\mathcal{H}'$ is itself described by the tensor-product Hilbert space $\mathcal{H}\otimes\mathcal{H}'$. The definition of this space is rather technical, particularly in infinite dimensions [6]. In practice, though, is very

[6] We can go on with finite dimension. First, let us define a linear form on a Hilbert space $\mathcal{H}$ as an application $T:\mathcal{H}\to\mathbb{C}$ which is linear. The set of all these forms has naturally structure of vector space and it is called the dual space $\mathcal{H}^*$. Now, given a basis of $\mathcal{H}$, $\mathcal{B}=\{|\psi_n\rangle\}$, for each element of this basis, we can define the dual element $\langle\psi_n|$ which acts on $|\psi_m\rangle$ simply as $\langle\psi_n|\psi_m\rangle$. (As usual, its action on a generic vector space is obtained extending by linearity.) This is obviously linear and so it belongs to $\mathcal{H}^*$. It turns out that a basis of the dual space is simply given by $\mathcal{B}^*=\{\langle\psi_n|\}$. (So, in particular, both $\mathcal{H}$ and $\mathcal{H}^*$ have the same dimension.) One can equally well define the dual of the dual, which consists of linear applications that send linear forms to $\mathbb{C}$. But this is essentially $\mathcal{H}$. Indeed, for each vector in $\mathcal{B}$, we can simply define the application of $|\psi_n\rangle$ on a dual form $\langle\psi_m|$, again, as $\langle\psi_m|\psi_n\rangle$. Now, given $\mathcal{H}$ and $\mathcal{H}'$, we can define the set of all linear 2-forms $T:\mathcal{H}^*\times\mathcal{H}'^*\to\mathbb{C}$, a basis of which is given by the forms (associated to bases in $\mathcal{H}$ and $\mathcal{H}'$) $|\psi_n\rangle\otimes|\psi'_m\rangle$ which, on a generic vector $(\langle\psi|,\langle\psi'|)\in\mathcal{H}^*\times\mathcal{H}'^*$ act like $\langle\psi|\psi_n\rangle\langle\psi'|\psi'_m\rangle$. This space is what we call the tensor product $\mathcal{H}\otimes\mathcal{H}'$. It has naturally structure of Hilbert space, in which the scalar product is simply that ensuing from a particular basis. That is, if we take the basis $\{|\psi_n\rangle\otimes|\psi_m\rangle\}$, any other vector $|\psi\rangle\in\mathcal{H}\times\mathcal{H}'$ can be written as

$$|\psi\rangle = \sum_{n,m} c_{nm}|\psi_n\rangle\otimes|\psi_m\rangle\,.$$

simple. Assume $\{|\psi_n\rangle\}$ is a basis of $\mathcal{H}$, and $\{|\psi'_n\rangle\}$ is a basis of $\mathcal{H}'$. Then, a basis of the tensor product is simply $\{|\psi_n\rangle \otimes |\psi'_m\rangle\}$. (We'll omit the $\otimes$ hereafter.). Any $|\psi\rangle \in \mathcal{H} \otimes \mathcal{H}'$ can therefore be expressed as

$$|\psi\rangle = \sum_{nm} c_{nm} |\psi_n\rangle |\psi'_m\rangle \,.$$

The scalar product between vectors in the tensor product is trivial: One take the product of each component separately. For a particular example, take the scalar product of $\frac{1}{\sqrt{2}}(|+\rangle|+\rangle + |+\rangle|-\rangle)$ with $|+\rangle|-\rangle$. We have:

$$\frac{1}{\sqrt{2}}(\langle+|+\rangle\langle+|-\rangle + \langle+|+\rangle\langle-|-\rangle) = \frac{1}{\sqrt{2}}\langle+|+\rangle\langle--\rangle = \frac{1}{\sqrt{2}} \,.$$

Composite systems might involve different or identical particles. In this latter case, a state in which particle p is in $|\psi\rangle$ while particle p' is in $|\psi'\rangle$ must be identical to that in which p is in $|\psi'\rangle$ and p' in $|\psi\rangle$. This means that the corresponding composite state $|\psi\rangle \in \mathcal{H} \otimes \mathcal{H}'$ must be the same under the swapping of p and p':

$$|\psi, \psi'\rangle = e^{i\alpha} |\psi', \psi\rangle \,.$$

Note that we have explicitly indicated that, for the state to be the same, the vector before and after swapping can differ by a phase. Swapping again, we obtain:

$$|\psi, \psi'\rangle = e^{2i\alpha} |\psi, \psi'\rangle \Rightarrow e^{i\alpha} = \pm 1 \,.$$

Particles with $e^{i\alpha} = 1$ are called **bosons**; those with $e^{i\alpha} = -1$ are **fermions**.

There's a standard way, based on the permutation group, to build symmetric and anti-symmetric states from single-state particles. Say that, in a system of N identical particles, these are in states $|\psi_1\rangle$,$|\psi_2\rangle$,...,$|\psi_N\rangle$ (two or more of these can coincide). Then, a state symmetric under permutation of any of these N particles is:

$$|\psi_1 \psi_2 \cdots \psi_N\rangle_S = \mathcal{N} \sum_p |\psi_{p(1)}\rangle |\psi_{p(2)}\rangle \cdots |\psi_{p(N)}\rangle \,,$$

where $\mathcal{N}$ is a normalization constant and p runs over the $N!$ permutations of $(1, 2, ..., N)$.

Let's consider the simplest example, $N = 2$. The permutations are $(1, 2)$ (trivial one) and $(2, 1)$. We have:

$$|\psi_1 \psi_2\rangle_S = \mathcal{N}(|\psi_1\rangle|\psi_2\rangle + |\psi_2\rangle|\psi_1\rangle) \,.$$

It is trivial to see that $\mathcal{N} = 1/\sqrt{2}$.

Let's see a more elaborated example with $N = 3$. We have the permutations $(1, 2, 3)$ (trivial), $(1, 3, 2)$, $(2, 1, 3)$, $(2, 3, 1)$, $(3, 1, 2)$, $(3, 2, 1)$. So:

$$\begin{aligned} |\psi_1 \psi_2 \psi_3\rangle_S = \mathcal{N}(&|\psi_1\rangle|\psi_2\rangle|\psi_3\rangle + |\psi_1\rangle|\psi_3\rangle|\psi_2\rangle + |\psi_2\rangle|\psi_1\rangle|\psi_3\rangle \\ &|\psi_2\rangle|\psi_3\rangle|\psi_1\rangle + |\psi_3\rangle|\psi_1\rangle|\psi_2\rangle + |\psi_3\rangle|\psi_2\rangle|\psi_1\rangle) \,. \end{aligned} \tag{2.1}$$

Hence, the scalar product of two vectors $|\psi\rangle$ and $|\psi'\rangle$ is simply

$$\langle\psi|\psi'\rangle = \sum_{nm} c^*_{nm} c'_{nm} \,.$$

.

So $\mathcal{N} = 1/\sqrt{6}$. Note that, if two of the single-particle states were identical, say $|\psi_1\rangle = |\psi_2\rangle$, then the normalization constant changes:

$$|\psi_1\psi_1\psi_3\rangle_S = \frac{1}{\sqrt{3}}(|\psi_1\rangle|\psi_1\rangle|\psi_3\rangle + |\psi_1\rangle|\psi_3\rangle|\psi_1\rangle + |\psi_3\rangle|\psi_1\rangle|\psi_1\rangle\,.$$

Things are equally easy for fermions. In this case though, the sum runs over all permutations weighted by the permutation sign:

$$|\psi_1\psi_2\cdots\psi_N\rangle_A = \mathcal{N}\sum_p s(p)|\psi_{p(1)}\rangle|\psi_{p(2)}\rangle\cdots|\psi_{p(N)}\rangle\,.$$

In the simplest case, $s(1,2) = 1$, $s(2,1) = -1$. So:

$$|\psi_1\psi_2\rangle_A = \frac{1}{\sqrt{2}}(|\psi_1\rangle|\psi_2\rangle - |\psi_2\rangle|\psi_1\rangle\,.$$

If $|\psi_1\rangle = |\psi_2\rangle$, then $|\psi_1\psi_1\rangle_A = 0$, which is nothing but **Pauli exclusion principle**: No two identical fermions can be in the same state.

Example 4. Exchange symmetry

Pauli's exclusion principle has implications in tons of areas of physics (atomic and molecular structure, solid state physics, ...). One simple yet interesting effect is what is known as **exchange symmetry**. Consider two identical particles moving in one dimension, described by wavefunctions $\psi_1(x_1)$ and $\psi_2(x_2)$ (let's assume they correspond to orthogonal states, e.g. different energy levels).

We can now compute the expectation value of $(x_1 - x_2)^2$, which provides indication of the relative location of both particles:

$$\langle(x_1 - x_2)^2\rangle_\psi = \langle x_1^2\rangle_\psi + \langle x_2^2\rangle_\psi - 2\langle x_1x_2\rangle_\psi\,.$$

In particles are distinguishable, then $\psi(x_1, x_2) = \psi_1(x_1)\psi_2(x_2)$. In this case:

$$\langle x_1^2\rangle_\psi = \int dx_1 x_1^2|\psi_1(x)|^2\int dx_2|\psi_2(x)|^2 = \langle x^2\rangle_{\psi_1}\,.$$

Likewise,

$$\langle x_2^2\rangle_\psi = \langle x^2\rangle_{\psi_2}\,,$$

and

$$\langle x_1x_2\rangle_\psi = \langle x\rangle_{\psi_1}\langle x\rangle_{\psi_2}\,.$$

Altogether:

$$\langle(x_1 - x_2)^2\rangle_\psi = \langle x^2\rangle_{\psi_1} + \langle x^2\rangle_{\psi_2} - 2\langle x\rangle_{\psi_1}\langle x\rangle_{\psi_2}\,.$$

If particles are identical, then the total wavefunction must be then:

$$\psi(x_1, x_2) = \frac{1}{\sqrt{2}}(\psi_1(x_1)\psi_2(x_2) \pm \psi_2(x_1)\psi_1(x_2))\,.$$

In this case, we have:

$$\begin{aligned}\langle x_1^2\rangle_\psi &= \frac{1}{2}\Big[\int dx_1 x_1^2|\psi_1(x_1)|^2\int dx_2|\psi_2(x_2)|^2+\int dx_1 x_1^2|\psi_2(x_1)|^2\int dx_2|\psi_1(x_2)|^2\\ &\pm\int dx_1 x_1^2\psi_1(x_1)^*\psi_2(x_1)\int dx_2\psi_2(x_2)^*\psi_1(x_2)\\ &\pm\int dx_1 x_1^2\psi_2(x_1)^*\psi_1(x_1)\int dx_2\psi_1(x_2)^*\psi_2(x_2)\Big]\\ &= \frac{1}{2}(\langle x^2\rangle_{\psi_1}+\langle x^2\rangle_{\psi_2})\,, \end{aligned} \tag{2.2}$$

because the last two term vanish since they involve the scalar product of $\psi_1(x)$ and $\psi_2(x)$ which are different elements of a basis.

The rest of the terms can be equally well computed, obtaining:

$$\langle(x_1-x_2)^2\rangle_\psi = \langle x^2\rangle_{\psi_1}+\langle x^2\rangle_{\psi_2}-2\langle x\rangle_{\psi_1}\langle x\rangle_{\psi_2}\mp|\langle x\rangle_{\psi_1\psi_2}|^2$$

where

$$\langle x\rangle_{\psi_1\psi_2}\equiv\int dx x\psi_1(x)^*\psi_2(x)\,.$$

So identical bosons tend to be closer, while identical fermions tend to be more separated. So this exchange-symmetry behaves *like* a force (though it is of course not a proper force).

Note that all this is relevant if particle wavefunctions actually overlap. Otherwise $\langle x\rangle_{\psi_1\psi_2}=0$. So for all practical purposes, separated particles can be treated as distinct.

2.2.1 "Derivation" of the Born rule

Justifying the third postulate needs further elaboration. This is about making sense of those states $|\psi\rangle$ which are not eigenstates of a given observable A. What can be said then about the value of A if the system is in the state $|\psi\rangle$? To answer this question, let me focus on the simplest yet completely comprehensive example. This is a 2-dimensional system spanned by eigenstantes $\{|+\rangle,|-\rangle\}$ of of some operator A; meaning $A|\pm\rangle=\pm|\pm\rangle$.

Let us take an arbitrary linear combination of these states, namely $|\psi\rangle=a|+\rangle+b|-\rangle$, with $a^2+b^2=1$. What we can prove is that, if we have a huge number N of copies of the same system in the state $|\psi\rangle$, then it is certain that the result of averaging the measurements of A in all systems is a^2-b^2, which is precisely the result we would expect under a probabilistic interpretation, because $\langle A\rangle_\psi=P(+)(+1)+P(-)(-1)=a^2-b^2$.

This average is itself an observable, which is naturally described by

$$\overline{A}=\frac{1}{N}\sum_i A^{(i)}\,.$$

So, what we have to do is simply showing that the state $|\psi^N\rangle=|\psi\rangle|\psi\rangle\cdots|\psi\rangle$, which represents the collective state of the full system, is an eigenstate of $\overline{A}$ with eigenvalue a^2-b^2 when $N\to\infty$. To this aim, we will rather show that $\langle\bar{A}\rangle^2_{\psi^N}-\langle\bar{A}^2\rangle_{\psi^N}$ vanishes for large N.

So, let us first compute $\langle\bar{A}\rangle_{\psi^N}=\langle\psi^N|\bar{A}|\psi^N\rangle$. This is

$$\frac{1}{N}\sum_i(a\langle+|+b\langle-|)\otimes\cdots\otimes(a\langle+|+b\langle-|)A^{(i)}(a|+\rangle+b|-\rangle)\otimes\cdots\otimes(a|+\rangle+b|-\rangle)\,.$$

Notice that $A^{(i)}$ simply changes the sign in front of b in the i-th ψ, which, when multiplied with its homologous bra, gives $a^2 - b^2$, while all other products are simply $a^2 + b^2 = 1$. Hence:

$$\langle \bar{A} \rangle_{\psi^N} = \frac{1}{N} \sum_i (a^2 - b^2) = \frac{1}{N}(a^2 - b^2) \sum_i 1 = \frac{N}{N}(a^2 - b^2) = a^2 - b^2 \,.$$

Let us now compute $\langle \bar{A}^2 \rangle_{\psi^N} = \langle \psi^N | \bar{A}^2 | \psi^N \rangle$. This is:

$$\frac{1}{N^2} \sum_{ij} (a\langle + | + b\langle - |) \otimes \cdots \otimes (a\langle + | + b\langle - | A^{(i)} A^{(j)} (a|+\rangle + b|-\rangle) \otimes \cdots \otimes (a|+\rangle + b|-\rangle) \,.$$

Now, if $i = j$, the action of $A^{(i)}A^{(j)}$ on the ket changes the sign of the i-th b twice, and hence it leaves it unaltered. The corresponding scalar product is thus 1. However, if $i \neq j$, both the i-th and the j-th b's change sign, given a total scalar product of $(a^2 - b^2)^2$. Thus, altogether, we have:

$$\langle \psi^N | \bar{A}^2 | \psi^N \rangle = \frac{1}{N^2} \sum_{ij} \delta_{ij} + \frac{1}{N^2}(a^2 - b^2)^2 \sum_{ij} \tilde{\delta}_{ij} \,,$$

where $\tilde{\delta}$ is the opposite of the δ, namely it gives 1 if $i \neq j$ and 0 otherwise. Hence:

$$\langle \psi^N | \bar{A}^2 | \psi^N \rangle = \frac{1}{N^2} N + \frac{1}{N^2}(a^2 - b^2)^2 N(N-1) \to (a^2 - b^2)^2$$

when $N \to \infty$.

After measurement, we encounter the "collpase" of the state vector. The collapse is simply the update of knowledge on the basis of new information. it is NOT a physical process. It is only the way we update probabilities based on new information.

2.2.2 Entanglement

Composite systems exhibit a very important property of QM, called entanglement. We say that two systems $\mathcal{H}$ and $\mathcal{H}'$ are entangled if the state $|\psi''\rangle \in \mathcal{H}'' = \mathcal{H} \otimes \mathcal{H}'$ of the composite system cannot be written as a tensor product of a vector $|\psi\rangle \in \mathcal{H}$ and another vector $|\psi'\rangle \in \mathcal{H}'$. Namely, $|\psi''\rangle \neq |\psi\rangle|\psi'\rangle$.

Examples: The state $|\psi\rangle = \frac{1}{\sqrt{2}}(|+\rangle|-\rangle + |-\rangle|-\rangle)$ is not entagled, as it's simply the product $\frac{1}{\sqrt{2}}(|+\rangle + |-\rangle) \otimes |-\rangle$. However, the following is an entangled state:

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|+\rangle|-\rangle - |-\rangle|+\rangle) \,.$$

How can we know whether a state is entangled? Define the **reduced density matrix**. Let $|\psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$. Then, the reduced density matrix for the system B is:

$$\rho_B = \mathrm{tr}_A[\rho] \equiv \sum_{\psi_A} \langle \psi_A | \rho | \psi_A \rangle \,,$$

where ψ_A runs over a basis of the first system and ρ is the density matrix of the full system. ρ_B is essentially the matrix defining the state of subsystem B ignoring all details about subsystem A.

Understanding this definition is simpler from a couple of examples.

First, let's assume $|\psi\rangle = |+\rangle_A|-\rangle_B \equiv |+-\rangle$. Then,

$$\rho = |+-\rangle\langle+-|\,.$$

So,

$$\rho_B = \mathrm{tr}_A[\rho] = \sum_{\psi_A}\langle\psi_A|+-\rangle\langle+-|\psi_A\rangle = \langle+|+\rangle|-\rangle\langle-| + 0 = |-\rangle_B\langle-|_B\,.$$

Second, consider $|\psi\rangle = \frac{1}{\sqrt{2}}(|++\rangle + |--\rangle)$. Then:

$$\rho = \frac{1}{2}(|++\rangle+|--\rangle)(\langle++|+\langle--|) = \frac{1}{2}(|++\rangle\langle++|+|++\rangle\langle--|+|--\rangle\langle++|+|--\rangle\langle--|)\,.$$

So,

$$\rho_B = \frac{1}{2}(|+\rangle\langle+| + |-\rangle\langle-|) = \frac{1}{2}\mathbb{I}\,.$$

Yet one more example: $|\psi\rangle = \frac{1}{\sqrt{2}}(|++\rangle + |+-\rangle)$. Then,

$$\rho = |\psi\rangle\langle\psi| = \frac{1}{2}(|++\rangle\langle++| + |++\rangle\langle+-| + |+-\rangle\langle++| + |+-\rangle\langle+-|)\,.$$

Hence:

$$\rho_B = \frac{1}{2}(|+\rangle\langle+| + |+\rangle\langle-| + |-\rangle\langle+| + |-\rangle\langle-|)\,.$$

Now, there's a theorem, that says that a state is entangled iff $\rho_B^2 = \rho_B$ (equivalently $\mathrm{tr}[\rho_B^2] \neq 1$). Thus, in the first case (trace is 1) the state is not entangled, the second one (trace is 1/2) the state is entangled, while the third one (trace 1) the state is again not entangled.

The proof is simple. First, let's note that an arbirary state $|\psi\rangle \in \mathcal{H}\otimes\mathcal{H}'$ can be written as

$$|\psi\rangle = \sum_{mn} c_{mn}|\psi_m\rangle|\psi'_n\rangle\,.$$

Now, using Singular-Value Decomposition, that is, the fact that a generic complex matrix C can be written as $C = UDV^\dagger$, with U and V unitary and D diagonal with entries $\sqrt{\lambda_i}$, we have:

$$|\psi\rangle = \sum_i \sqrt{\lambda_i}|\psi_i\rangle|\psi'_i\rangle$$

where $|\psi_i\rangle = \sum_m U_{mi}|\psi_m\rangle$ and $|\psi'_i\rangle = \sum_n V^*_{ni}|\psi_n\rangle$. The sum extends to r, which is the rank of C, and that's a basis invariant (this is important for the following discussion). And because U and V are unitary, the states $|\psi_i^{(\prime)}\rangle$ are form orthonormal bases too. So necessarily $\sum_i \lambda = 1$.

Take now the partial trace, we have

$$\rho_A = \mathrm{tr}_B[|\psi\rangle\langle\psi|] = \sum_i \lambda_i|\psi_i\rangle\langle\psi_i|\,.$$

So we encounter the same situation as in the case of determining whether the density matrix represents a pure state. If $\rho_A^2 = \rho$, then there's a single element in the sum, and hence the state is not entangled. Otherwise is entangled, because there can't be another

(not-entangled) basis in which the sum involves only one element because r is a basis invariant.

Entanglement implies that properties of subsystems are **correlated**. Formally, this means that the outcomes (probabilities of eigenvalues) of measurements performed on one of the systems depend on the information about the second system. This correlation works even among properties which are not well-defined, like in $\frac{1}{\sqrt{2}}(|++\rangle + |--\rangle)$ where the value (+ or −) of any of the subsystems is ill-defined (we only know that, upon measurement, it can be + or − with probability 1/2).

Correlation has nothing to do with effects from one system onto another. The measurement in one particle of an entangled system does **not** affect the other. There can be even no interaction Hamiltonian!

2.3 Quantum foundations

Entanglement and Hidden Variables

Entanglement implies that the state of each subsystem in a composite quantum system cannot be defined independently of the others. Nevertheless, there exist strong correlations between the properties of the subsystems.

For instance, consider the entangled state

$$|\psi\rangle = \frac{1}{\sqrt{2}}\big(|+-\rangle + |-+\rangle\big), \tag{2.1}$$

written in the basis of eigenstates of

$$A = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{2.2}$$

If we measure the observable A in the first subsystem, the probability of obtaining + or − is 1/2. Once the outcome is known—say, "+"—the wave function collapses to $|+-\rangle$. This immediately determines the result of measuring A in the second subsystem: it must be "−". Remarkably, this correlation persists even if the two subsystems are separated by kilometers.

At first sight, this may not seem surprising. Classically, we can imagine placing two balls—one black, one white—into separate boxes and sending them far apart. Before opening a box, the probability of finding either color is 1/2. Once we open one box and find, say, the black ball, we instantly know that the other contains the white one.

The striking quantum feature is that such correlations persist even for properties that cannot be simultaneously well defined. Consider the observable

$$B = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tag{2.3}$$

which also has eigenvalues ± 1 and eigenvectors $|\pm\rangle_B$. In the basis of B, the same state can be written as

$$|\psi\rangle = \frac{1}{\sqrt{2}}\big(|+-\rangle_B + |-+\rangle_B\big). \tag{2.4}$$

Thus, both observables A and B exhibit perfect correlations between the two subsystems—even though they do not commute, $[A, B] \neq 0$, and hence cannot have definite values simultaneously.

This deeply puzzled many physicists, including Einstein, who argued that quantum mechanics must be incomplete. According to this view, the situation should be analogous to the classical balls: the apparent randomness of measurement outcomes merely reflects our ignorance of some deeper *hidden variables* that, if known, would allow perfect prediction of all results. In such a framework, all physical quantities would be well defined at all times, and quantum mechanics would be just an effective description.

However, as later shown by Bell's theorem and subsequent experiments, this hidden-variable interpretation cannot reproduce all quantum predictions—proving that nature itself does not behave in a purely classical, deterministic way.

2.3.1 CHSH inequality and GHZ states

The best experiment I know of to prove that one can not safely assign simulateneous values to properties represented by non-commuting observables is the so-called GHZ. This consists in three entangled particles described by:

$$|\psi\rangle = \frac{1}{2}(|++\rangle - |--\rangle)\,.$$

And we have the observables

$$A = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, B = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, C = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\,.$$

We will prove that: (1) The product of measurements of C in two systems and B in the other is always $+1$. (2) The product of measurements of B in the three systems is necessarily -1. (3) That this is impossible in a classical theory where all properties are well-defined.

Note that (1) and (2) hold even though individual measurements in each sub-system are random.

We only need to prove, first, that $C^{(i)}C^{(j)}B^{(k)}|\psi\rangle = \psi$ for $(i, j, k) = (1, 2, 3), (1, 3, 2), (2, 3, 1)$. (Note that these operators commute because they act on different Hilbert spaces.) This is trivial. Second, we need to prove that $B^{(1)}B^{(2)}B^{(3)}|\psi\rangle = -\psi$. Equally trivial.

Now, assume the hidden-variables perspective. Then, the particles have definite values of B and C, even though we supposedly don't know them. But there's a finite number of possibilities: $\frac{J_x}{J_y} = \frac{+++}{+++}$, $\frac{+++}{---}$, ... None of this fullfills both that the product CCB is $+1$ and BBB is -1.

We'll see in the next section that the correct (meaning, in agreement with experiment) result is the QM one. Still, some people don't want to give up classical physics yet. So they propose to (more or less crazy) possibilities to explain this result in classical terms (namely, assuming B and C are well defined simultaneously):

1. Action at a distance: One might be tempted to say that measuring one particle somehow affects the others instantaneously, even before any measurement is performed on them. The problem with this interpretation is that, when the particles are widely separated (as confirmed in experiments), such an influence would have to propagate faster than light, in clear violation of relativity. And violating relativity would in turn lead to a host of further inconsistencies throughout physics.

2. Superdeterminism: This affirms that the experimenter is not free to measure CCB or BBB for any state $|\psi\rangle$. This theory has the problem that it essentially breaks science, since it amounts to say no two different hypotheses cannot be tested.

2.3.2 Quantum computing

Which one is right? This has been long a hard-to-answer question, which at the end resulted in several Nobel prizes. Today, however, we can simply check with a quantum computer. This is simply a system composed of several qbits (2-dim quantum systems).

We'll use the IBM quantum computer: https://quantum-computing.ibm.com/ .

In it, we first construct the the GHZ state starting from a $|000\rangle$ state. To do so one can only apply unitary operations (quantum gates), because that's how systems evolve in time in QM ($e^{-iHt/\hbar}$ is unitary). The way is first using Hadamard gate on the first qbit. In the basis $\{|0\rangle, |1\rangle\}$ it is defined by:

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \tag{2.5}$$

which is obviously unitary: $H^\dagger = H^{-1} = H$. We have:

$$H_1|000\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)|00\rangle = \frac{1}{\sqrt{2}}(|000\rangle + |100\rangle)\,.$$

Now we should apply a CNOT gate between the first and second qbits. This gate is given, in the basis $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$ by:

$$\text{CNOT} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}\,.$$

Which is obviously unitary (is block-diagonal with identity and parity). This essentially changes the second qubit iff the first qubit is 1. So:

$$\frac{1}{\sqrt{2}}(|000\rangle + |100\rangle) \to \frac{1}{\sqrt{2}}(|000\rangle + |110\rangle)\,.$$

Applying CNOT one last time between the first and third qbits, one obtains the GHZ state.

The next step is measuring C of two qbits and B of the other, which we choose randomly. Then we measure B of all particles and make the product.

2.4 Exercises

Exercise 2.4.1 *Consider a physical system with Hilbert space spanned by two orthonormal vectors, $\{|a_1\rangle, |a_2\rangle\}$. The state of the system is $|\psi\rangle = \frac{1}{2}(|a_1\rangle + \sqrt{3}|a_2\rangle)$. The system does not evolve in time.*

1. *What is the probability of obtaining $|a_1\rangle$ in two consecutive observations of the state of the system?*
2. *What is the probability of obtaining the same state in two consecutive observations?*
3. *The state of the system is observed. What is the probability of obtaining the same state in a subsequent observation?*

Solution. Notice first that it is here implicit that "measuring the state of the system" amounts to measuring the observable A of which a_1 and a_2 are eigenvalues. Please get use to this little abuse of language. (In general, the probability that a system in the state $|\psi\rangle$ is found in $|\psi'\rangle$ after observation is $|\langle\psi'|\psi\rangle|^2$.)

The probability of obtaining $|a_1\rangle$ in a first observation is

$$P = \left(\frac{1}{2}\right)^2 = \frac{1}{4}\,.$$

After this, the system remains in the state $|a_1\rangle$, so a second observation reveals $|a_1\rangle$ with certainty. Therefore, the probability of obtainig $|a_1\rangle$ after two consecutive observations of the state of the system is simply

$$P = \frac{1}{4} \times 1 = \frac{1}{4}\,.$$

About the second point, in either case ($|a_1\rangle$ or $|a_2\rangle$), the system remains in the observed state. So the probability of obtaining the same state in two consecutive observations is $P = 1$.

For the third point, similarly to the previous reasoning, we can conclude that $P = 1$.

Exercise 2.4.2 *Consider a non-hermitian operator A which, however, commutes with its adjoint. Find some relation between the eigenvalues of A and $A^\dagger$ on common eigenvectors, as well as between the scalar product of two eigenstates of A with different eigenvalues.*

Solution. A is not hermitian, so $A \neq A^\dagger$. However, $[A, A^\dagger] = 0$. Let's call $|\psi\rangle$ any of the common eigenvectors. Then,

$$A|\psi\rangle = a|\psi\rangle\,, \quad A^\dagger|\psi\rangle = b|\psi\rangle\,.$$

We have the following identities:

$$\langle\psi|AA^\dagger|\psi\rangle = b^*b = |b|^2\,, \tag{2.1}$$

$$\langle\psi|A^\dagger A|\psi\rangle = a^*a = |a|^2\,, \tag{2.2}$$

$$\langle\psi|AA^\dagger|\psi\rangle = b\langle\psi|A|\psi\rangle = ba\,. \tag{2.3}$$

Since the two operators commute, the three equalities must be the same. Namely: $a^*a = ab$, $b^*b = ab$ and hence $a^* = b$.

Say now that $|\psi'\rangle$ is an eigenvector with different eigenvalue. Then,

$$\langle\psi'|A|\psi\rangle = a\langle\psi'|\psi\rangle = b'^*\langle\psi'|\psi\rangle$$

and hence $(a - a')\langle\psi'|\psi\rangle = 0$. Since $a \neq a'$, the two eigenvectors are orthogonal.

Exercise 2.4.3 *Consider two different eigenvectors $|\psi\rangle$ and $|\psi'\rangle$ of a unitary operator U with eigenvalues λ and λ', respectively. What is the relation between these eigenvalues if the two states are not orthogonal?*

Solution. The unitary operator U satisfies $U^\dagger U = 1 = UU^\dagger$. We also have that $U|\psi\rangle = \lambda|\psi\rangle$ and $U|\psi'\rangle = \lambda'|\psi'\rangle$. Then,

$$\langle\psi|\psi'\rangle = \langle\psi|U^\dagger U|\psi'\rangle = \lambda'\langle\psi|U^\dagger|\psi'\rangle = \lambda'\lambda^*\langle\psi|\psi'\rangle\,.$$

And so, $(\lambda'\lambda^* - 1)\langle\psi|\psi'\rangle = 0$, implying $\lambda'\lambda^* = 1$.

Likewise,

$$\langle\psi|\psi\rangle = \langle\psi|U^\dagger U|\psi\rangle = |\lambda|^2\langle\psi|\psi\rangle\,,$$

from where $|\lambda|^2 = 1$. We can similarly obtain $|\lambda'|^2 = 1$. Altogether, we have that $\lambda = \lambda' = e^{i\alpha}$.

Exercise 2.4.4 *Consider a system in which two observables A and B commute with the Hamiltonian as follows: $[H, A] = i\omega B$, $[H, B] = -i\omega A$, with $\omega \in \mathbb{R}$. Suppose that the expectations values of A and B are known at $t = 0$. Compute the expectation values of these quantities at $t > 0$.*

Solution. In Heseinberg's picture,

$$\dot{A} = \frac{i}{\hbar}[H, A]$$

and likewise for B. So,

$$\dot{A} = \frac{i}{\hbar}i\omega B = -\frac{\omega}{\hbar}B\,.$$

(A very common mistake at this stage is integrating this equation as if B was time-independent, namely obtaining $A(t) = -\frac{\omega}{\hbar}Bt + \mathrm{c}$.)

Taking the time derivative of both $\dot{A}$ and $\dot{B}$, we find:

$$\ddot{A} = -\frac{\omega^2}{\hbar^2}A\,, \tag{2.4}$$

$$\ddot{B} = -\frac{\omega^2}{\hbar}B\,; \tag{2.5}$$

from where we get:

$$A(t) = \mathrm{c}_1 \sin\frac{\omega}{\hbar}t + \mathrm{c}_2\cos\frac{\omega}{\hbar}t\,, \tag{2.6}$$

$$B(t) = \mathrm{c}_3 \sin\frac{\omega}{\hbar}t + \mathrm{c}_4\cos\frac{\omega}{\hbar}t\,. \tag{2.7}$$

Taking the derivative of these equations, we find the original ones iff $c_4 = -c_1$, $c_3 = c_2$. Altogether, we find:

$$\langle A(t)\rangle = \langle A(0)\rangle \cos\frac{\omega}{\hbar}t - \langle B(0)\rangle \sin\frac{\omega}{\hbar}t\,, \tag{2.8}$$

$$\langle B(t)\rangle = \langle B(0)\rangle \cos\frac{\omega}{\hbar}t + \langle A(0)\rangle \sin\frac{\omega}{\hbar}t\,. \tag{2.9}$$

Exercise 2.4.5 *The Hamiltonian of a system is given in the basis* $\mathcal{B} = \{|11\rangle, |10\rangle, |1-1\rangle\}$ *of eigenstates of certain operator* S *by the matrix*

$$H = \frac{E_0}{4}\begin{pmatrix} 2 & -\sqrt{2} & -i\sqrt{2} \\ -\sqrt{2} & 3 & -i \\ i\sqrt{2} & i & 3 \end{pmatrix}.$$

1. *Are the observables* H *and* S *compatible? What are the possible values of the energy?*
2. *If the system is in the lower energy state and we measure* S*, what is the probability to obtain* 0*?*
3. *Suppose we take a sequential measurement of the energy,* S *and again the energy starting in an arbitrary initial state. Is it possible that the sequence gives the values* E_{min}*,* 0*,* E_{max}*? If yes, what is the final state?*

Exercise 2.4.6 *Consider a normalised state* $|\psi\rangle$ *at* $t = 0$ *and define*

$$\Delta E = \sqrt{\langle (H - \langle H\rangle_\psi)^2\rangle_\psi}\,.$$

Calculate the probability that the system remains in state $|\psi\rangle$ *after a short time* δt*, expressing the result in terms of* ΔE*,* $\hbar$ *and* δt *to second order in* δt*.*

Solution. Unitary evolution gives

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

Expanding the exponential to order δt^2 we find:

$$|\delta(t)\rangle = (1 - \frac{i}{\hbar}H\delta t - \frac{1}{2\hbar^2}H^2\delta t^2)|\psi\rangle = |\psi\rangle - \frac{i}{\hbar}\delta t H|\psi\rangle - \frac{\delta t^2}{2\hbar^2}H^2|\psi\rangle\,.$$

The probability of remaining in the state $|\psi\rangle$ after δt is given by

$$\begin{aligned} P = |\langle\psi(\delta t)|\psi\rangle|^2 &= \left|\langle\psi|\psi\rangle - \frac{i}{\hbar}\delta t\langle\psi|H|\psi\rangle - \frac{\delta t^2}{2\hbar^2}\langle\psi|H^2|\psi\rangle\right|^2 \\ &= 1 + \frac{i}{\hbar}\delta t\langle\psi|H|\psi\rangle - \frac{\delta t^2}{2\hbar^2}\langle\psi|H^2|\psi\rangle \\ &- \frac{i}{\hbar}\delta t\langle\psi|H|\psi\rangle - \frac{\delta t^2}{2\hbar^2}\langle\psi|H^2|\psi\rangle + \frac{\delta t^2}{\hbar^2}\langle\psi|H|\psi\rangle^2 + \mathcal{O}(\delta t^3) \\ &= 1 + \frac{\delta t^2}{\hbar^2}\langle H\rangle_\psi^2 - \frac{\delta t^2}{\hbar^2}\langle H^2\rangle_\psi\,. \end{aligned} \tag{2.10}$$

Now,

$$(\Delta E)^2 = \langle (H - \langle H\rangle_\psi)^2\rangle_\psi = \langle H^2\rangle_\psi + 2\langle H\rangle_\psi^2 - \langle H\rangle_\psi^2\,, \tag{2.11}$$

and so

$$P = 1 - \frac{\delta t^2}{\hbar^2}(\Delta E)^2\,.$$

Exercise 2.4.7 *Consider a quantum system with 3-dimensional Hilbert space. The matrices of the Hamiltonian H and some other observable A in the basis $\{|u_1\rangle, |u_2\rangle, |u_3\rangle$ are given by*

$$H = \hbar\omega \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}\,, \quad A = a \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}\,.$$

Initially the system described by the state $|\psi\rangle = c(|u_1\rangle + \frac{1}{2}|u_2\rangle + \frac{1}{2}|u_3\rangle$, with c some normalisation constant.

(a) Find the expectation value of A at time $t = 0$. If we measure A at $t = 0$, what are the possible outcomes and probabilities?

(b) Suppose we measure A at time $t = 0$ and obtain $-a$. What values can be obtained if we later measure the energy and with what probabilities? Do these depend on time? What is the expectation value of the energy at $t \geq 0$?

(c) Find the density matrix describing the state of the system before and right after measuring A to all the elements of an ensemble in the pure state $|\psi\rangle$, if the result of the measurement of A is unknown.

Solution. Let's first write $|\psi\rangle$ in a normalized way and in components:

$$|\psi\rangle = \sqrt{\frac{2}{3}}(1, \frac{1}{2}, \frac{1}{2})\,.$$

Thus, we simply have:

$$\langle A\rangle_\psi = \frac{2}{3}a(1, \frac{1}{2}, \frac{1}{2}) \begin{pmatrix} \frac{1}{2} \\ 1 \\ -\frac{1}{2} \end{pmatrix} = \frac{a}{2}\,.$$

We can also do it in explicit dyad form, with $A = a(|u_1\rangle\langle u_2| + |u_2\rangle\langle u_1| - |u_3\rangle\langle u_3|)$:

$$\begin{aligned} \langle\psi|A|\psi\rangle &= \frac{2}{3}a(\langle u_1| + \frac{1}{2}\langle u_2| + \frac{1}{2}\langle u_3|)A(|u_1\rangle + \frac{1}{2}|u_2\rangle + \frac{1}{2}|u_3\rangle) \\ &= \frac{2}{3}a(\frac{1}{2}\langle u_1|u_1\rangle\langle u_2|u_2\rangle + ...) = \frac{a}{2}\,. \end{aligned} \tag{2.12}$$

To know the possible values of measuring A, we compute the eigenvalues. One is obvious, $-a$. The others are also easy because A is already block-diagonal:

$$\det \begin{pmatrix} -\lambda & 1 \\ 1 & -\lambda \end{pmatrix} = 0 \Rightarrow \lambda = \pm 1$$

in units of a, so $\lambda = \pm a$. So $-a$ is degenerated.

To get the probabilities, we need to know the eigenspaces. One eigenvector is obvious, $|-a_1\rangle = (0,0,1)$. It has eigenvalue $-a$. The other eigenstate with eigenvalue $-a$ must live in the subspace span$\{|u_1\rangle, |u_2\rangle\}$. Let's find it:

$$a\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}x\\ y\end{pmatrix} = -a\begin{pmatrix}a\\ y\end{pmatrix} \Rightarrow y = -x\,.$$

So, we have $|-a_2\rangle = \frac{1}{\sqrt{2}}(-1,1,0)$. Finally, the eigenvector with eigenvalue a must be orthogonal to both, so $|a\rangle = \frac{1}{\sqrt{2}}(1,1,0)$.

Given that we'll have to work with both A and H, and because they commute, is better to find a common basis of eigenvectors. It should be clear that these three vectors are also eigenvectors of H (any linear combination of $|u_1\rangle$ and $|u_2\rangle$ is, and A and H share $|u_3\rangle$). Altogether, we can label the basis of the Hilbert space using the eigenvalues of A (in units of a) and H (in units of $\hbar\omega$):

$$|2-1\rangle = (0,0,1)\,, \quad |11\rangle = (1,1,0)\,, \quad |1-1\rangle = \frac{1}{\sqrt{2}}(-1,1,0)\,.$$

We say that $\{A, H\}$ form a CSCO. A by itself is not, nor is H.

Now, to know the probabilities, we write $|\psi\rangle$ in terms of eigenvectors of A:

$$|\psi\rangle = \frac{\sqrt{3}}{2}|11\rangle + \frac{1}{2\sqrt{3}}|1-1\rangle + \frac{1}{\sqrt{6}}|2-1\rangle\,.$$

This form shows explicitly the decomposition of $|\psi\rangle$ into the subsapce of eigenvalue a and that of eigenvalue $-a$.

So, the probability of obtaining a is $p_a = 3/4$. And hence $p_{-a} = 1/4$.

Now, if we obtain $-a$, then the state collapses to $|\psi\rangle \to \frac{1}{2\sqrt{3}}|1-1\rangle + \frac{1}{\sqrt{6}}|2-1\rangle$, but properly normalized! That is:

$$|\psi\rangle \to \frac{1}{\sqrt{3}}(|1-1\rangle + \sqrt{2}|2-1\rangle)\,.$$

It is this state that we now have to consider when measuring H. We have $p_{\hbar\omega} = 1/3$, $p_{2\hbar\omega} = 2/3$.

The eigenvalues of H do not change with time (obviously), nor their probabilities. So the expectation value is $\langle H\rangle_\psi = 1/3 + 2\times 2/3 = 5/3\hbar\omega$.

If we later measure A, nothing changes either (because A and H commute!). If we measure H, we have to collapse to the corresponding eigenspace, and that affects later measurements of H (but not of A; because we're already in a single eigenvalue eigenspace).

Exercise 2.4.8 *A particle of mass m and charge q is described by the Hamiltonian*

$$H = -\vec{\mu} \cdot \vec{B}\,, \quad \vec{\mu} = \frac{q}{m}\vec{S}\,.$$

At $t = 0$, the particle is in a state such that $\langle S_y \rangle = \hbar/4$, $\langle S_x \rangle = \langle S_z \rangle = 0$, where

$$S_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\,, \quad S_y = \begin{pmatrix} o & -i \\ i & 0 \end{pmatrix}\,, \quad S_z = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\,.$$

1. *Is that a pure or a mixed state?*
2. *What are the possible outcomes and probabilities of measuring S_y?*
3. *Find $\langle S_x \rangle$ and $\langle S_z \rangle$ at arbitrary times.*

Exercise 2.4.9 *Consider a particle moving over a one-dimensional circumference of radius R, described by the Hilbert space of periodic functions $f(x + 2\pi R) = f(x)$.*

1. *Show that the momentum operator $P[f(x)] = -if'(x)$, which acts over periodic functions f, is hermitian.*
2. *Find the spectrum of P.*
3. *Show that the position operator $X[f(x)] = xf(x)$ is not well defined.*

Solution. The scalar product within this Hilbert space is given by $\langle f|g\rangle = \int_0^{2\pi R} dx f(x)^* g(x)$.

For the first part, it suffices to prove that $\langle g|P|f\rangle = \langle g|P^\dagger|f\rangle$. By definition of hermitian, he RHS of this equality reads:

$$\begin{aligned}
\langle g|P^\dagger|f\rangle = \langle f|P|g\rangle^* &= i\hbar \int_0^{2\pi R} dx f(x) g^{*\prime}(x) \\
&= i\hbar \int_0^{2\pi R} dx \left[(fg^*)'(x) - f'(x)g^*(x)\right] \\
&= i\hbar \left[f(x)g^*(x)\right]_0^{2\pi R} - i\hbar \int_0^{2\pi R} dx g^*(x) f'(x) \\
&= -i\hbar \int_0^{2\pi R} dx g^*(x) f'(x)\,. \qquad (2.13)
\end{aligned}$$

And this is clearly $\langle g|P|f\rangle$.

To find the spectrum, we just impose $P|p\rangle = p|p\rangle$, which reads:

$$-i\hbar p'(x) = pp(x)$$

from where $p(x) = Ne^{\frac{i}{\hbar}px}$. The normalization constant N can be obtained upon enforcing

$$\langle p|p\rangle = N^2 \int_0^{2\pi R} dx = 1 \Rightarrow N = \frac{1}{2\pi R}\,.$$

Since $p(0) = p(2\pi R)$, then $e^{\frac{i}{\hbar}p2\pi R} = 1$ and so $p = n\hbar/R$ with n integer.

Finally, it is trivial to show that $Xf(x) = xf(x)$ is not periodic, so it takes vectors out the Hilbert space.

Exercise 2.4.10 *Show that there is a single energy eigenstate for a particle subject to the one-dimensional potential $V(x) = -V_0\delta(x)$.*

Solution. Let us first integrate Schrödinger's equation over a small range $[-\epsilon, \epsilon]$:

$$-\frac{\hbar^2}{2m}\int_{-\epsilon}^{\epsilon} dx\psi''(x) = \int_{-\epsilon}^{\epsilon} dx(E + V_0\delta(x))\psi(x)\,.$$

Taking the limit of small ϵ, we arrive at:

$$\lim_{\epsilon\to 0}(\psi'(x)|_{\epsilon} - \psi'(x)|_{-\epsilon}) = -\frac{2mV_0}{\hbar^2}\psi(0)\,,$$

from where we see that, unlike what occurs, for example, in the finite-well potential, here the derivative of the wavefunction is itself discontinuous (at the origin). The wavefunction itself must be continuous, though.

This implies that the solution of negative energy (bound state) must have the form

$$\psi(x) = \begin{cases} \mathrm{c}e^{\eta x}, x < 0 \\ \mathrm{c}e^{-\eta x}, x > 0 \end{cases},$$

where $\mathrm{c} = \psi(0)$.

Hence, the discontinuity in the derivative is

$$\lim_{\epsilon\to 0}(\psi'(x)|_{\epsilon} - \psi'(x)|_{-\epsilon}) = -2\mathrm{c}\eta\,,$$

and therefore $\eta = \frac{mV_0}{\hbar^2}$. The energy is given by

$$E = -\frac{\hbar^2\eta^2}{2m} = -\frac{V_0^2 m}{2\hbar^2}\,.$$

Exercise 2.4.11 *A system of two particles, each of them described by a Hilbert space with basis $\mathcal{B} = \{|+\rangle, |-\rangle\}$, is initially in the state*

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|+-\rangle + |-+\rangle)\,.$$

The Hamiltonian of the system is $H = \lambda S_{x_1} \otimes S_{z_2}$, where

$$S_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad S_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad S_z = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

(a) Find the state of the system at a time t. You can use that

$$e^{i\theta S_i \otimes S_j} = \cos\theta + iS_i \otimes S_j \sin\theta\,.$$

(b) Are S_{z_1} and S_{z_2} compatible with H? What about the sum of both?

(c) Find the reduced density matrix of the first particle at a time t. Is there any t for which this density matrix describes a pure state?

□ The first part is trivial, since $S_z|\pm\rangle = \pm|\pm\rangle$ and $S_x|\pm\rangle = |\mp\rangle$. So:

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}}\left[\cos\frac{\lambda t}{\hbar}(|+-\rangle + |-+\rangle - i\sin\frac{\lambda t}{\hbar}(|++\rangle - |--\rangle)\right].$$

The commutators are equally trivial:

$$[H, S_{z_1}] = \lambda[S_{x_1}, S_{z_1}] \otimes S_{z_2} \neq 0\,, \quad [H, S_{z_2}] = \lambda S_{x_1} \otimes [S_{z_2}, S_{z_2}] = 0\,.$$

So only S_{z_2} is compatible with H. The sum is obviously not either.

For the reduced density matrix, we have:

$$\langle +_2|\psi(t)\rangle\langle\psi(t)|+_2\rangle = \frac{1}{2}(c|-\rangle - is|+\rangle)(is\langle +| + c\langle -|) = \frac{1}{2}\begin{pmatrix} s^2 & -isc \\ isc & c^2 \end{pmatrix},$$
$$\langle -_2|\psi(t)\rangle\langle\psi(t)|-_2\rangle = \frac{1}{2}\begin{pmatrix} c^2 & -ics \\ ics & s^2 \end{pmatrix}. \qquad (2.14)$$

So:

$$\rho_1(t) = \frac{1}{2}\begin{pmatrix} 1 & -2ics \\ 2ics & 1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & -i\sin\frac{2\lambda t}{\hbar} \\ i\sin\frac{2\lambda t}{\hbar} & 1 \end{pmatrix},$$

The state is pure when $\mathrm{tr}[\rho_1^2(t)] = [1 + \sin^2(2\lambda t/\hbar)]/2 = 1$.

Chapter 3

Symmetries

3.1 Symmetries

What are the observables in QM? It is usual to "borrow" them from their classical analogues. This has two problems, though. First, QM is more fundamental than classical mechanics, so it should be a way to build observables without resorting on classical physics. Second, there're QM observables which do not have classical analogue; e.g. the spin. What we will see is that relevant observables are generators of symmetries.

An example of symmetry is rotational invariance of a sphere. The set of all symmetries g form a group: there is g^{-1}, there is e and gg' is another symmetry.

Laws of Nature are invariant under symmetries. This is a tremendously important (and powerful!) observation. Have you ever thought why Newton's force is Gmm'/r^2 and Coulomb's one is Cqq'/r^2? Why are they essentially the same? The reason is that, to be rotationally invariant, $F(\vec{x}) = F(r)$; this r itself must be difference between two positions to be traslational invariant; moreover F can not depend explicity on t or otherwise time translational invariance $t \to t + \tau$ wouldn't hold. I view this statement as more fundamental than physics itself, almost necessary for this to be science. If laws of physics were dependent on time or space, how could we check predictions?

A symmetry doesn't leave the coordinates invariant (think for example a rotation). Likewise, symmetries don't necessarily leave state vectors invariant. However, the transition probabilities must remain invariant.

This implies, $|\psi\rangle \to |\psi\rangle'$ such that $|\langle\psi'|\phi'\rangle|^2 = |\langle\psi|\phi\rangle|^2$. (Actually is a bit more complicated, because it should transform is rays into rays.) An obvious way to do this is via a linear unitarity operator, $|\psi\rangle' = U|\psi\rangle$. Indeed, $\langle\psi'|\phi'\rangle = \langle\psi|U^\dagger U|\phi\rangle = \langle\psi|\phi\rangle$ if $U^\dagger U = 1$. Or in other words, $U^\dagger = U^{-1}$.

Wigner showed that this is one of the only two possibilities; the other one is represented by antilinear and anti-unitary operators, namely

$$U(\alpha|\psi\rangle + \alpha'|\psi'\rangle) = \alpha^* U|\psi\rangle + \alpha'^* U|\psi'\rangle$$

and

$$\langle\psi|U^\dagger U|\phi\rangle = \langle\psi|\phi\rangle^* .$$

In practice, we'll be mostly interested on unitarity operators. Note that, $\mathbb{I}$ is unitarty; if U_1 and U_2 are unitary, then $U_1 U_2$ is unitary (indeed, $(U_1U_2)^\dagger(U_1U_2) = U_2^\dagger U_1^\dagger U_1 U_2 = U_2^\dagger U_2 = 1$); if U is unitary, then U^{-1} is unitary (trivial). Hence, the set of unitarity operators from a group. Actually, a representation of a group. We'll be mostly interested on those that represent continous groups of symmetries, like translations or rotations.

In such cases, we can make transformations that depart from the identity as little as we want:

$$U(\epsilon) = 1 + i\epsilon T + \mathcal{O}(\epsilon^2)\,.$$

Unitarity then implies

$$(1 - i\epsilon T^\dagger + ...)(1 + i\epsilon T + ...) = 1 \Rightarrow T = T^\dagger\,.$$

Consersely, we can exponentiate T to obtain $U(\theta)$ irrespective of proximity to the identity: $U(\theta) = e^{i\theta T}$.

We can see symmetry transformations to act not on states, but rather on observables. To see how, let's consider the transformation of the expectation value:

$$\langle A\rangle_\psi \to \langle\psi|A|\psi\rangle = \langle\psi|U^{-1}AU|\psi\rangle\,.$$

This is equivalent to assuing vectors stay invariant and operators transform as $A \to U^{-1}AU$. This is called the **Heisenberg Picture**, in contrast with Schrödinger's picture where state change and operators stay.

The transformation $A \to U^{-1}AU$ is called a **similarity transformation**. It preserves multiplication and addition: $AB \to U^{-1}AB$, $A + B \to U^{-1}(A + B)U$. Most importantly, it can be seen that eigenvalues of A are not modified by symmetry transformations. Indeed, let's assume $A|a\rangle = a|a\rangle$. We can insert the identity between A and $|a\rangle$ in the form of $U^{-1}U$ and multiply everything on the left by U^{-1}:

$$U^{-1}AUU^{-1}|a\rangle = aU^{-1}|a\rangle\,.$$

This implies that the transformed operator, $U^{-1}AU$ has en eigenvector $U^{-1}|a\rangle$ with eigenvalue a. So the possibles values of observables are the same in all "reference systems". However, the probabilities don't need to (think simply of a system on a state $|x\rangle$, under a translation the system goes to $|x + a\rangle$).

Let's go back now to symmetry transformation close to the identity. We have $U = 1 + i\epsilon T$. So,

$$A \to U^{-1}AU = (1 - i\epsilon T)(1 + i\epsilon T) = A + i\epsilon[A, T].$$

This means, the commutator between the generators of the symmetry and the observable determine whether this changes or not.

3.2 Time and space translations

Time translations

Time translations are transformations of the form $t \to t+\tau$. Obviously the set of all these is a continuous (τ is a real parameter) group which is abelian (commutative). They're tehrefore represented by unitarity operators $U(\tau)$:

$$U(\tau)|\psi(t)\rangle = |\psi(t + \tau)\rangle\,.$$

We can obtain $U(\tau)$ upon exponentiating the generator H of the symmetry (by definition, we call this the Hamiltonian):

$$e^{-i\frac{H}{\hbar}\tau}|\psi(t)\rangle = |\psi(t + \tau)\rangle\,.$$

In particular, for $t = 0$,

$$|\psi(\tau)\rangle = e^{-i\frac{H}{\hbar}\tau}|\psi(0)\rangle \Rightarrow \frac{d}{d\tau}|\psi(\tau)\rangle = -i\frac{H}{\hbar}e^{-i\frac{H}{\hbar}\tau}|\psi(0)\rangle = -i\frac{H}{\hbar}|\psi(\tau)\rangle$$

and so

$$i\hbar\frac{d}{dt}|\psi\rangle = H\psi\,,$$

which is nothing but Schrodinger's equation.

Under time translations, any observable A evolves as $A \to A + \frac{it}{\hbar}[H, A]$, or in other words

$$\dot{A}(t) = \frac{i}{\hbar}[H, A]\,.$$

(Note the similarily with classical physics in Poisson-bracket form: $f'(t) = \{f, H\}$.)

Hence, if $[H, A] = 0$, A is conserved.

Space translations

Let's consider the position operator, $X|x\rangle = x|x\rangle$ and hence $X|x + a\rangle = (x + a)|x + a\rangle$. This latter state is the result of translating $|x\rangle$ using a (unitarity representation of a) space translation $U(a)$:

$$XU(a)|x\rangle = (x + a)U(a)|x\rangle \Rightarrow U^{-1}(a)XU(a)|x\rangle = (x + a)|x\rangle\,.$$

And because the $|x\rangle$ span a basis of the Hilbert space, we can say that $U^{-1}(a)XU(a) = X + a$. (The operator a is simply a multiplied by the identity.)

Take now $U(a) = 1 - \frac{i}{\hbar}Pa$, where P is by definition the momentum operator. We have:

$$(1 + \frac{i}{\hbar}Pa)X(1 - \frac{i}{\hbar}Pa) = X + a \Rightarrow X + \frac{i}{\hbar}[Pa, X] = X + a$$

and so

$$[P, X] = -i\hbar$$

which is nothing but Heisenberg's uncertainty principle.

If we work on 3 dimensions and with N particles, we would obtain

$$[X_{ni}, P_{mj}] = i\hbar\delta_{nm}\delta_{ij}\,.$$

The generator of the symmetry, the full momentum operator, is

$$\vec{P} = \sum_n \vec{P}_n\,.$$

This is the actual generator of translations. Particle by particle, namely $\vec{P}_n$ in isolation, is meaningless. (Component by component though, namely $\vec{P}_i$ is the generator of translation in a particular direction.)

The question we want to address is how these generators commute. To this aim, let's first notice that the translation group is commutative, and hence $U(\vec{b})U(\vec{a}) = U(\vec{b})U(\vec{a})$. Expanding this around the identity (small $\vec{a}$ and $\vec{b}$), but in this case we need to go to second order!:

$$(1 - \frac{i}{\hbar}\vec{P}\vec{a})(1 - \frac{i}{\hbar}\vec{P}\vec{b}) = (1 - \frac{i}{\hbar}\vec{P}\vec{b})(1 - \frac{i}{\hbar}\vec{P}\vec{a}) \Rightarrow \vec{P}\vec{a}\vec{P}\vec{b} = \vec{P}\vec{b}\vec{P}\vec{a}$$

which implies

$$\sum_{ij} P_i a_i P_j b_j = \sum_{ij} P_j b_j P_i a_i \Rightarrow P_i P_j a_i b_j = P_j P_i b_j a_i \Rightarrow [P_i, P_j] = 0\,.$$

Wavefunction representation

We can now introduce the notion of wavefunction and derive how P acts on this new object. To this aim, let's first notice that x is a continuos parameter. So what we have is $1 = \int dx|x\rangle\langle x|$. Hence,

$$|\psi\rangle = \int dx|x\rangle\langle x|\psi\rangle = \int dx\psi(x)|x\rangle\,.$$

So, by definition, $\psi(x) = \langle x|\psi\rangle$. One can prove that this way, scalar product and probabilities and so on work as seen in quantum physics course.

Also, $\langle x|x'\rangle = \delta(x - x')$, because otherwise introducing the identity would not work:

$$\langle x'|\psi\rangle = \int dx\langle x'|x\rangle\langle x'\psi\rangle = \int dx\delta(x' - x)\langle x|\psi\rangle = \langle x'|\psi\rangle\,.$$

With this information, we can now derive the wavefunction representation of the position operator:

$$X|\psi\rangle = X\int dx|x\rangle\langle x|\psi\rangle = \int dxX|x\rangle\psi(x) \Rightarrow \langle x'|X|\psi\rangle = x'\psi(x')\,.$$

[Much simpler, simply apply X to bra.]

Now inspect P, let's act with $U = \exp(-iaP/\hbar)$ on $|\psi\rangle$:

$$U|\psi\rangle = U\int dx|x\rangle\langle x|\psi\rangle = \int dx|x + a\rangle\langle x|\psi\rangle$$

which, doing the change of variables $x' = x + a$ (and then renaming x' to x) reads:

$$U|\psi\rangle = \int dx|x\rangle\langle x - a|\psi\rangle = \int dx\psi(x - a)|x\rangle\,.$$

Notice now that, for small a, $\psi'(x) = 1/a(\psi(x+a)-\psi(x))$ and so $\psi(x-a) \sim \psi(x)-a\psi'(x)$. Therefore:

$$(1 - \frac{ia}{\hbar}P)|\psi\rangle = \int dx\psi(x)|x\rangle - a\int dx\psi'(x)|x\rangle = |\psi\rangle - a\int dx\,\psi'(x)|x\rangle\,.$$

Multiplying with $\langle x'|$:

$$-\frac{ia}{\hbar}\langle x'|P|\psi\rangle = -a\int dx\psi'(x)\langle x'|x\rangle = -a\psi'(x') \Rightarrow P\psi(x) = -i\hbar\frac{d}{dx}\psi(x)\,.$$

From there one can trivially check that $[X, P]\psi(x) = i\hbar\mathbb{I}$.

3.3 Rotations

Rotations are (particular types of) linear transformations that take a vector $\vec{x}$ into $R\vec{x}$ and that leave the scalar product of vectors invariant: $\vec{x}\cdot\vec{y} = (R\vec{x})\cdot(R\vec{y})$. In index notation, $R_{ij}x_jR_{ik}y_k = x_iy_i$, where summation over repeated indices (Einstein's convention) is implied. This has to hold for arbitrary x and y, which implies (simply apply the equation above to $x_i = \delta_{ia}$ and $y_i = \delta_{ib}$:

$$R_{ij}R_{ik} = \delta_{jk}\,.$$

Or, in matrix notation, $R^T R = 1$. Matrices that fulfill this condition are called **orthogonal**. The set of all orthogonal matrices in d dimensions is called $O(d)$.

Note that $\det(R^T R) = \det(R^T)\det(R) = \det^2(R) = 1$ and so $\det(R) = \pm 1$. This implies that R are invertible, and from the condition $R^T R = 1$ it is clear that $R^- = R^T$. Obviously, R^{-1} is also orthogonal, and morevoer, if $R_1, R_2 \in O(d)$, then $R_1 R_2 \in O(d)$. Simply compute $(R_1 R_2)^T (R_1 R_2) = R_2^T R_1^T R_1 R_2 = 1$.

So $O(d)$ is a group. Now, not all elements of $O(d)$ are rotations. For example, in three dimensions the transformation $\vec{x} \to -\vec{x}$ is an inversion. Its main characteristic is that is has determinant -1. The elements $A \in O(d)$ with $\det(A) = -1$ do not form a subgroup (the identity is not in there!). Rotations are those elements with unit determinant and they do form a (continous) group called $SO(d) = \{R \in O(d)/\det(R) = 1\}$ or **special orthogonal** group.

$SO(3)$ is probably one of the most important groups in high-energy physics. The reason is that $SO(3)$ represents 3d rotations, but on top of this is (locally) isomorphic to $SU(2)$, which describes aproximately the symmetries of strong interactions (isospin), moreover the Lorentz group is a essentially $SU(2) \times SU(2)$ and even more the electroweak symmetry is described by $SU(2)$.

On the Hilbert space, rotations R are represented, as usual, by unitarty operators $U(R)$, so that

$$U(R_1)U(R_2) = U(R_1 R_2)\,.$$

On vector operators such as X or P, rotations act like [1]

$$U^{-1}(R) V_i U(R) = R_{ik} V_k\,.$$

From here, we can obtain how a vector operator V commutes with the generators of the rotations (the angular momenta J_{ij}). To this aim, we consider a small rotation $R = 1 + \omega + \mathcal{O}(\omega^2)$ with $\omega^T = -\omega$. To first order in ω we have

$$U(R) = U(1+\omega) = 1 + \frac{i}{2\hbar}\omega_{kl} J_{kl}\,.$$

Plugging this expression into the equation above, we find:

$$(1 - \frac{i}{2\hbar}\omega_{kl} J_{kl}) V_i (1 + \frac{i}{2\hbar}\omega_{kl} J_{kl}) = R_{ik} V_k = (\delta_{ik} + \omega_{ik}) V_k = V_i + \omega_{ik} V_k$$

which implies

$$V_i - \frac{i}{2\hbar}\omega_{kl} J_{kl} V_i + \frac{i}{2\hbar}\omega_{kl} J_{kl} = V_i + \omega_{ik} V_k$$

and so

$$-\frac{i}{2\hbar}\omega_{kl}[J_{kl}, V_i] = \omega_{ik} V_k\,.$$

[1] A different way of seeing this is the following: $U(R)|\vec{x}\rangle = |R\vec{x}\rangle$. Hence,

$$\vec{X}U(R)|\vec{x}\rangle = (R\vec{x})|R\vec{x}\rangle \Rightarrow U^{-1}(R)\vec{X}U(R)|\vec{x}\rangle = U^{-1}(R)(R\vec{x})|R\vec{x}\rangle = (R\vec{x})U^{-1}(R)|R\vec{x}\rangle = (R\vec{X})|\vec{x}\rangle\,.$$

Since this holds for all elements $|\vec{x}\rangle$ of a basis, then

$$U^{-1}(R)\vec{X}U(R) = R\vec{X}\,.$$

We would like to obtain an expression not involving ω. So we should factor the same factor of ω on both sides. For this matter, note that $\omega_{ik} = \delta_{il}\omega_{lk}$, and so $\omega_{ik}V_k = \delta_{il}\omega_{lk}V_k = \omega_{kl}V_l\delta_{ik}$, where in the last equality we have simply renamed dummy indices. Hence:

$$-\frac{i}{2\hbar}\omega_{kl}[J_{kl}, V_i] = \omega_{kl}V_l\delta_{ik}\,.$$

However, we can not yet say that, because this equation holds for all values of ω, we can simply equate the corresponding coefficients. THis is so because ω is not fully arbitrary, but rather constrained by $\omega_{ji} = -\omega_{ij}$. What we can do, however, is writting without loss of generality $\omega_{ij} = \alpha_{ij} - \alpha_{ji}$, where α is completely arbitrary. This implies:

$$-\frac{i}{2\hbar}(\alpha_{kl} - \alpha_{lk})[J_{kl}, V_i] = (\alpha_{kl} - \alpha_{lk})V_l\delta_{ik}$$

and so

$$-\frac{i}{\hbar}\alpha_{kl}[J_{kl}, V_i] = \alpha_{kl}\delta_{ik}V_l - \alpha_{lk}V_l\delta_{ik} = \alpha_{kl}(\delta_{il}V_l - \delta_{il}V_k)$$

and now we can equatate coefficients of α:

$$\frac{i}{\hbar}[J_{kl}, V_i] = -\delta_{ik}V_l + \delta_{il}V_k\,.$$

If we're precisely in 3 dimensions, then J_{ij} contains only three independent operators, which we can choose as $J_1 \equiv J_{23}$, $J_2 \equiv J_{31}$, $J_3 \equiv J_{12}$. (In this new variables, a small rotation reads $U(1+\omega) = 1 + \frac{i}{\hbar}\vec{\omega}\cdot\vec{J}$ where now $\vec{\omega}$ is a three-component object, completely arbitrary, that parametrises and angle $|\vec{\omega}|$ around $\vec{\omega}$. In terms of these new expressions, we have that the equation above reads:

$$[J_i, V_j] = i\hbar\epsilon_{ijk}V_k\,.$$

For example, $[J_1, V_2] = [J_{23}, V_2] = i\hbar V_3$.

We would like now to see how the angular momenta themselves commute, first in general dimensions and then particularising to $d = 3$. To this aim, let's consider the following rotation:

$$U(R'^{-1})U(1+\omega)U(R') = U(R'^{-1}(1+\omega)R') = U(1 + R'^{-1}\omega R)$$

which is valid for any (antisymmetric) ω and any rotation R' independent of ω. TO first order in ω, we have (factors of $i\hbar$ and the identity cancel in each side):

$$\omega_{ij}U(R'^{-1})J_{ij}U(R') = (R'^{-1}\omega R')_{kl}J_{kl} = (R'^{-1})_{ki}\omega_{ij}R'_{jl}J_{kl} = R'_{ik}R'_{jl}\omega_{ij}J_{kl}\,.$$

Equating both components of ω (conveniently written as a difference of arbitrary α's, but here doesn't make a change):

$$U(R'^{-1})J_{ij}U(R') = R'_{ik}R'_{jl}J_{kl}\,.$$

Notice that J changes like a vector in each index. It is a tensor. But this doesn't tell us yet how the $J's$ commute. To obtain this, we need to go a step further and make R itself small, $R' = 1 + \omega'$. We have:

$$(1-\frac{i}{2\hbar}\omega'_{kl}J_{kl})J_{ij}(1+\frac{i}{2\hbar}\omega'_{kl}J_{kl}) = (\delta_{ik}+\omega'_{ik})(\delta_{jl}+\omega'_{jl})J_{kl} \Rightarrow J_{ij}+\frac{i}{2\hbar}[J_{ij}, \omega'_{kl}J_{kl}] = \omega'_{ik}J_{kj}+\omega'_{jl}J_{il}$$

and again this holds for all values of $\omega = -\omega^T$.

If we use again the trick $\omega = \alpha - \alpha^T$, we end up with:

$$\frac{i}{\hbar}[J_{ij}, J_{kl}] = -\delta_{il}J_{kj} + \delta_{ik}J_{ij} + \delta_{jk}J_{il} - \delta_{jl}J_{ik}\,.$$

And this hold in arbitrary space dimension. For three dimensions, we have:

$$[J_i, J_j] = i\hbar\epsilon_{ijk}J_k\,.$$

This is the same commutation relation as that satisfied by $\vec{L}$! We, again, have obtained it from first principles.

It also tells us that $\vec{J}$ is a vector. (Not surprising because $J_k = \frac{1}{2}\epsilon_{ijk}J_{ij}$, which is the contraction of two tensors.)

Let's consider the orbital angular momentum, $\vec{L} = \vec{X} \times \vec{P}$. It can be checked by explicit computation that

$$[L_i, L_j] = i\hbar\epsilon_{ijk}L_k$$

. Moreover, it can be easily seen (is an exercise) that the cross product of vector operators is a vector too. Hence,

$$[J_i, L_j] = i\hbar\epsilon_{ijk}L_k\,.$$

Therefore, if we define $\vec{S} \equiv \vec{J} - \vec{L}$, which is another vector operator, then by substracting the two equations above we get

$$[J_i, L_j] - [L_i, L_j] = [S_i, L_j] = 0$$

. So:

$$[S_i, S_j] = [J_i - L_i, S_j] = [J_i, S_j] - [L_i, S_j] = i\hbar\epsilon_{ijk}S_k - 0\,.$$

And so $\vec{S}$ is another angular momentum. This is called the spin. It is completely independent of position and momentum. In fact, it commutes with them. It can be checked this simply because, by explicit computation, $[L_i, X_j] = i\hbar\epsilon_{ijk}X_k$ and likewise for P_j. But X and P are vector operators and so commute alike with J. So $[S_i, X_j] = [S_i, P_j] = 0$. But we have derived this independence without relying on any notion of having a separate Hilbert space of different degree of freedom or anything like that.

Spectrum of angular momenta

We would like to compute the eigenvectors and eigenvalues of $\vec{J}^2 = J_iJ_i$ and J_3 in any algebra $[J_i, J_j] = i\hbar\epsilon_{ijk}J_k$.

We notice first that $\vec{J}^2$ commutes with all $\vec{J}$. Let's imply check the $[\vec{J}^2, J_3]$:

$$[\vec{J}^2, J_3] = [J_1^2, J_3] + [J_2^2, J_3] + [J_3^2, J_3] = ... = 0\,.$$

Because of these, we can search for common eigenvectors $|jm\rangle$ of both, where $J_3|jm\rangle = \hbar m|jm\rangle$ while the we leave the action of $\vec{J}^2$ unspecified. Let's now consider the following commutator:

$$[J_3, J_1 \pm iJ_2] = [J_3, J_1] \pm i[J_3, J_2] = i\hbar J_2 \pm i(-i\hbar J_1) = \pm\hbar(J_1 \pm iJ_2)\,.$$

We'll often write $J\pm = J_1 \pm iJ_2$. From here, it follows that:

$$J_3J_\pm|jm\rangle = [J_3, J_\pm]|jm\rangle + J_\pm J_3|jm\rangle = \pm\hbar J_\pm|jm\rangle + \hbar m J_\pm|jm\rangle = \hbar(m \pm 1)J_\pm|jm\rangle\,.$$

This implies that $J_\pm|jm\rangle$ is an eigenstate of J_3 with eigenvalue $\hbar(m\pm1)$. Moreover, given that $J_\pm|jm\rangle$ doesn't change the eigenvalue under $\vec{J}^2$ (this and $J_\pm$ commute, so the space of eigenvectors of $\vec{J}^2$ with given eigenvalue is invariant under the action of $J_\pm$), we can say that $J_\pm|jm\rangle \sim |jm\pm1\rangle$.

If we take an arbitray $|jm\rangle$ and keep applying J_+, we get eigenvectors with larger and larger eigenvalues of J_3. Likewise, if we apply consequetevely J_-, we obtain eigenvectors with smaller and smaller eigenvalues. The list of all vectors of this kind must be finite, though. This can be proven as follows. Say the eigenvalues of $|\psi\rangle$ for $\vec{J}^2$ and J_3 are a and b, respectively. Then:

$$a - b^2 = \langle\psi|(\vec{J}^2 - J_3^2)|\psi\rangle = \langle\psi|(J_1^2 + J_2^2)|\psi\rangle \geq 0\,.$$

So because all elements on the multiplet that can be formed by applying $J_\pm$ to $|jm\rangle$ have the same j, there must be a maximum (and a minimum) value under J_3 or otherwie the inequality above would be broken. Let's call them j' and j''. This means:

$$(J_1 + iJ_2)|j'\rangle = 0\,, \quad (J_1 - iJ_2)|j''\rangle = 0\,. \tag{3.1}$$

Also, we know that we go from j'' to j' by applying $J_\pm$ an integer number of times, so

$$j' - j'' \in \mathbb{N}\,.$$

Our final aim is understanding how $\vec{J}^2$ as well as J_1 and J_2 (or equivalently $J_\pm$) act exactly on the states $|jm\rangle$. To this aim, we need this intermediate result:

$$J_-J_+ = J_1^2 + iJ_1J_2 - iJ_2J_1 + J_2^2 = J_1^2 + J_2^2 + i[J_1, J_2] = \vec{J}^2 - J_3^2 - \hbar J_3\,, \tag{3.2}$$

$$J_+J_- = \vec{J}^2 - J_3^2 + \hbar J_3\,. \tag{3.3}$$

So,

$$J_-J_+|j'\rangle = 0 = \vec{J}^2|j'\rangle - J_3^2|j'\rangle - \hbar J_3|j'\rangle \Rightarrow \vec{J}^2|j'\rangle = \hbar^2 j'(j'+1)|j'\rangle\,.$$

Likewise,

$$J_+J_-|j''\rangle = \hbar^2 j''(j''-1)|j''\rangle\,.$$

But both $|j'\rangle$ and $|j''\rangle$ have the same eigenvalue of $\vec{J}^2$, implying that

$$j'(j'+1) = j''(j''-1) \Rightarrow j''^2 - j'' - j'^2 - j' = 0 \Rightarrow j'' = -j'\,.$$

because the other solution, namely $j'' = 1 + j'$ is non-valid (we know that $j'' < j'$). This, together with the fact that $j' - j'' \in \mathbb{N}$, implies that $j = n/2$ with $n \in \mathbb{N}$.

Altogether, we have:

$$J_3|jm\rangle = \hbar m|jm\rangle\,, \tag{3.4}$$

$$\vec{J}^2|jm\rangle = \hbar^2 j(j+1)|jm\rangle\,; \tag{3.5}$$

with $m = -j, -j+1, ..., j$.

Necessarily, $\langle jm|jm'\rangle = 0$ for $m \neq m'$ (because these are eigenstates of the same operator with different eigenvalue). Moreover, if we scale appropriately $|jm\rangle$, we can get $\langle jm|jm'\rangle = \delta_{mm'}$.

Finally, let's see how $J_\pm$ act on the different states. We have that:

$$J_+|jm\rangle = \alpha^+(j,m)|jm+1\rangle\,.$$

But also $J_-J_+ = \vec{J}^2 - J_3^2 - \hbar J_3$ and so:

$$\langle jm|J_-J_+|jm\rangle = |\alpha^+(j,m)|^2 = \hbar^2 j(j+1) - \hbar m^2 - \hbar m\,.$$

By choosing appropriately phases for $|jm\rangle$, we can make $\alpha^\pm$ real and positive and hence:

$$\alpha^\pm(j,m) = \hbar\sqrt{j(j+1) - m^2 \mp m}\,.$$

In other words:

$$J_\pm|jm\rangle = \hbar\sqrt{j(j+1) - m^2 \mp m}|jm \pm 1\rangle\,.$$

A practical application of this result is the following. Consider two states $|jm\vec{\alpha}\rangle$ and $|jm\vec{\beta}\rangle$ where α and β label other quantum numbers. Then, the transition amplitude $\langle jm\vec{\alpha}|jm\vec{\beta}\rangle$ does not depend on m. Or in other words, is the same for m as for $m+1$. Indeed:

$$\begin{aligned}\langle jm+1\vec{\alpha}|jm+1\vec{\beta}\rangle &= \frac{1}{\hbar^2\sqrt{j(j+1)-m^2-m}}\langle jm+1\vec{\alpha}|J_+|jm\vec{\beta}\rangle \\ &= \frac{\hbar^2\sqrt{j(j+1)-(m+1)^2+(m+1)}}{\hbar^2\sqrt{j(j+1)-m^2-m}}\langle jm\vec{\alpha}|jm\vec{\beta}\rangle \\ &= \langle jm\vec{\alpha}|jm\vec{\beta}\rangle\,. \end{aligned} \tag{3.6}$$

Likewise, $\langle jm\vec{\alpha}|A|jm\vec{\beta}\rangle$ is m-independent whenever $[A,\vec{J}] = 0$.

The Hydrogen atom

There is a way, using only the algebra of angular momenta, of obtaining the spectrum of the Hydrogen atom (in the absence of spin):

$$H = \frac{\vec{P}^2}{2m} - \frac{Ze^2}{r}\,.$$

The idea consists in finding an operator $\vec{A} = f(H)$ dependent on the Hamiltonian (remember that we can define functions of operators via $f(A)|\psi\rangle = f(A)(\sum_i c_i|a_i\rangle) = \sum_i c_i f(a_i)|a_i\rangle$), that reproduces the algebra of $SU(2)$ and that commutes with H. Thus, in the basis of common eigenvectors of $\vec{A}^2$ and H, we have

$$\vec{A}^2|aE\rangle = \hbar^2 a(a+1)|aE\rangle = f(E)|aE\rangle$$

so that inverting the relation we get the values of the energies.

This derivation is due to Pauli. It is based on the Runge-Lenz vector:

$$\vec{R} = -\frac{Ze^2\vec{X}}{r} + \frac{1}{2m}(\vec{P}\times\vec{L} - \vec{L}\times\vec{P})\,.$$

It is clear that $\vec{R}$ is a vector operator. Note that we symmetrize the second term to make $\vec{R}$ Hermitian (classically there's no different between $\vec{P}\times\vec{L}$ and $-\vec{L}\times\vec{P}$). Indeed:

$$(\vec{L}\times\vec{P})_i = \epsilon_{ijk}L_jP_k \Rightarrow (\vec{L}\times\vec{P})_i^\dagger = \epsilon_{ijk}P_k^\dagger L_j^\dagger = \epsilon_{ijk}P_kL_j = -\epsilon_{ikj}P_kL_j = -\epsilon_{ijk}P_jL_k = -(\vec{P}\times\vec{L})_i\,. \tag{3.7}$$

We can actually refine this relation (using $[L_i, p_j] = i\hbar\epsilon_{ijk}p_k$ because angular momentum):

$$\begin{aligned}(\vec{L}\times\vec{P})_i &= \epsilon_{ijk}L_jP_k = \epsilon_{ijk}([L_j,P_k]+P_kL_j)\\ &= \epsilon_{ijk}(i\hbar\epsilon_{jkm}P_m + P_kL_j)\\ &= i\hbar\epsilon_{kij}\epsilon_{kmj}P_m - \epsilon_{ikj}P_kL_j\\ &= i\hbar(\delta_{im}\delta_{jj}-\delta_{ij}\delta_{jm})P_m - (\vec{P}\times\vec{L})_i\\ &= i\hbar(3P_i - P_j\delta_{ij}) - (\vec{P}\times\vec{L})_i = 2i\hbar P_i - (\vec{P}\times\vec{L})_i\\ &\Rightarrow \frac{1}{2m}(\vec{P}\times\vec{L}-\vec{L}\times\vec{P}) = \frac{1}{2m}(-2i\hbar\vec{P}+2\vec{P}\times\vec{L}) = \frac{1}{m}\vec{P}\times\vec{L} - \frac{i\hbar}{m}\vec{P}\,. \end{aligned} \quad (3.8)$$

Why we want $\vec{R}$ to be hermitian will become clearer later. Classically $\vec{R}$ si conserved (for the Coulomb potential as well as for the hamornic oscillator. As a consequence, bounded orbits are closed. (Things change in General Relativity, since at weak gravity the Newtonian potential gets corrections which are not Coulomb-like. This explains Mercury's anomalous perihelion.)

Quantum mechanically, we have that $[H,\vec{R}] = 0$. Note that the Hamiltonian commutes also with $\vec{L}$, because the potential is spherically symmetric and in the absence of spin the total angular momentum is simply $\vec{L}$. Now, upon using the relation above for $(\vec{L}\times\vec{P})_i$, we can rewrite $\vec{R}$ as

$$\vec{R} = -\frac{Ze^2\vec{X}}{r} + \frac{1}{2m}(\vec{P}\times\vec{L}-\vec{L}\times\vec{P}) = -\frac{Ze^2\vec{X}}{r} + \frac{1}{m}\vec{P}\times\vec{L} - \frac{i\hbar}{m}\vec{P}\,.$$

From here, it is straightforward though extremely lengthy to obtain:

$$\vec{R}^2 = Z^2e^2 + \left(\frac{2H}{m}\right)(\vec{L}^2+\hbar^2)\,.$$

From here, it is also easy but very tedious to obtain:

$$[R_i,R_j] = -\frac{2i}{m}\hbar\epsilon_{ijk}HL_k \Rightarrow [\frac{R_i}{\sqrt{H}},\frac{R_j}{\sqrt{H}}] = \frac{2i}{m}\hbar\epsilon_{ijk}L_k\,.$$

Moreover, because $\vec{R}$ is a vector operator,

$$[L_i,R_j] = i\hbar\epsilon_{ijk}R_k\,.$$

So, $\vec{R}/\sqrt{H}$ and $\vec{L}$ form a closed algebra, meaning that the commutator of any two of them is a linear combinations of them themselves. The miracoulous thing is that this algebra is isomorphic to $SU(2)\times SU(2)$. To see this, let us define:

$$\vec{A}_\pm \equiv \frac{1}{2}(\vec{L}\pm\sqrt{\frac{m}{-2H}}\vec{R})\,.$$

We have then:

$$\begin{aligned}[A_{+i},A_{-j}] &= \frac{1}{4}[L_i+\sqrt{\frac{m}{-2H}}R_i, L_j-\sqrt{\frac{m}{-2H}}R_j]\\ &= \frac{1}{4}\{[L_i,L_j] - \sqrt{\frac{m}{-2H}}[L_i,R_j] + \sqrt{\frac{m}{-2H}}[L_i,R_j] - \frac{m}{2H}[R_i,R_j]\}\\ &= \frac{i\hbar}{4}\{\epsilon_{ijk}L_k - \sqrt{\frac{m}{-2H}}\epsilon_{ijk}R_k + \sqrt{\frac{m}{-2H}}\epsilon_{ijk}R_k - \frac{m}{2H}\frac{2}{m}\epsilon_{ijk}L_k\} = 0\,. \end{aligned} \quad (3.9)$$

One can likewise obtain

$$[A_{\pm i}, A_{\pm j}] = i\hbar\epsilon_{ijk}A_{\pm k}\,,$$

which shows that we have two $SU(2)$ algebras. However, because $\vec{L}\cdot\vec{R} = \vec{R}\cdot\vec{R} = 0$, we have that

$$\vec{A}_+^2 = \vec{A}_-^2 \equiv \vec{A}^2 = \frac{1}{4}(\vec{L}^2 + \frac{m}{-2H}\vec{R}^2)\,.$$

And of course we have $[\vec{A}^2, H] = 0$. So we can find common eigenstates of $\vec{A}^2$ and H, which we name $|aE\rangle$. From our knowledge on angular momentum, we know that

$$\vec{A}^2|aE\rangle = \hbar^2 a(a+1)|aE\rangle\,, \quad E < 0\,.$$

This is because if $E > 0$ then $\vec{A}$ is not hermitian! So applying simply our results above we obtain:

$$\begin{aligned}\vec{A}^2|aE\rangle = \hbar^2 a(a+1)|aE\rangle &= \frac{1}{4}(\vec{L}^2 + \frac{m}{-2E}\vec{R}^2)|aE\rangle \\ &= \frac{1}{4}\left[\vec{L}^2 + \frac{m}{-2E}Z^2e^4 - (\vec{L}^2 + \hbar^2)\right]|aE\rangle \\ &= -\frac{m}{8E}Z^2e^4 - \frac{\hbar^2}{4} \Rightarrow -\frac{m}{8E}Z^2e^4 = \frac{\hbar^2}{4}(2a+1)^2 \equiv \frac{\hbar^2}{4}n^2\,.\end{aligned} \tag{3.10}$$

And hence

$$E_n = -\frac{Z^2e^4m}{2\hbar^2n^2}\,.$$

The degeneracy of each of this energy levels is clear: For each a, $\vec{A}_\pm$ can take $(2a+1)$ values, and so there're $(2a+1)^2 = n^2$ different states for each E_n. Though not immediate, these n^2 states can be labeled by $\ell = 0, 1, ...n-1$ and $m_\ell = -\ell, ..., \ell$. As a cross-check, note that

$$\sum_{\ell=0}^{n-1}(2\ell+1) = 2\sum_{\ell=0}^{n-1}\ell + n = 2\sum_{i=1}^{n}(i-1) + n = 2\sum_{i=1}^{n}i - 2\sum_{i=1}^{n}1 + n \tag{3.11}$$

$$= n(n+1) - 2n + n = n^2\,. \tag{3.12}$$

If we include the spin, but ignore terms in the Hamiltonian associated to it, then the states with energy E_n can be labeled as $|n\ell s, m_\ell m_s\rangle$ and the degeneracy of E_n is twice larger, corresponding to $m_s = -1/2, 1/2$. We could equally well described the states with energy E_n using the basis $|n\ell sjm\rangle$ with $j = \ell - 1/2, \ell + 1/2$.

The names for states with $\ell = 0, 1, 2, ...$ are $s, p, d, ...$ historically originated in "sharp", "principal", "diffuse", etc. corresponding to how clear spectral lines between originated in transitions involving the corresponding states looked like. (One could wonder why ℓ matters for how these lines look like, if energies depend only on n. The reason is that, in the presence of finer interactions, like spin-orbit coupling or magnetic fields, energies depend also on ℓ and even maybe other quantum numbers.) So, in the abscence of other interactions, the states of the Hydrogen-like atoms are (ignoring m_ℓ): $1s$, $2s$ and $2p$, $3s, 3p, 3d$, ...

Addition of angular momenta

We might have different angular momenta involved in the same problem, $\vec{J}'$ and $\vec{J}''$, $[J'_i, J''_j] = 0$. We could work with common eigenstates of both, that we name $|j'j'', m'm''\rangle$. However, sometimes is easier to work in a basis in which instead $\vec{J}'^2$, $\vec{J}''^2$, $\vec{J}^2$ and J_3 are well defined, with $\vec{J} = \vec{J}' + \vec{J}''$. One example is when the Hamiltonian involves terms of the type $\vec{L} \cdot \vec{S} = \vec{J}^2 - \vec{L}^2 - \vec{S}^2$.

Note that the operators $\vec{J}'^2$, $\vec{J}''^2$, $\vec{J}^2$ and J_3 they all commute among themselves, and of course $[J_i, J_j] = i\hbar\epsilon_{ijk}J_k$; common eigenvestors are named $|j'j''jm\rangle$, with:

$$\vec{J}'^2|j'j''jm\rangle = \hbar^2 j'(j'+1)|j'j''jm\rangle\,, \tag{3.13}$$

$$\vec{J}''^2|j'j''jm\rangle = \hbar^2 j''(j''+1)|j'j''jm\rangle\,, \tag{3.14}$$

$$... \tag{3.15}$$

So it should be possible to write the vectors in one basis as linear combinations of the others:

$$|j'j''jm\rangle = \sum_{m'm''} C_{j'j''}(jm, m'm'')|j'j'', m'm''\rangle\,, \tag{3.16}$$

with

$$c_{j'j''}(jm, m'm'') = \langle j'j'', m'm''|j'j''jm\rangle\,.$$

The $C's$ are called Clebsch-Gordan coefficients. Of course they non-vanishing only in some cases. For example, it is clear that $m' + m'' = m$:

$$\begin{aligned} 0 &= \langle j'j'', m'm''|J_3 - J'_3 - J''_3|j'j''jm\rangle \\ &= \langle j'j'', m'm''|J_3|j'j''jm\rangle - \langle j'j'', m'm''|(J'_3 + J''_3)|j'j''jm\rangle \\ &= (m - m' - m'')C_{j'j''}(jm, m'm'')\,. \end{aligned} \tag{3.17}$$

So the number of states in each basis *for a given* m is the same.

Now, what are the possible values of m if $m = m' + m''$? It must range from $m = -j' - j'', ..., j' + j''$. Therefore the maximum value is $j' + j''$. That should be also the maximum value of j, otherwise there'd be a higher m (associated to this higher j).

But this largest value of j and m happens only for the maximum $m' = j'$ and $m'' = j''$. There is only one possibility, meaning:

$$C_{j'j''}(jm, j'j'') = \delta_{j,j'+j''}\delta_{m,m'+m''}\,.$$

Let's see this clearer with an example: $j' = 1/2$, $j'' = 1$. We have six possibilities. [...]

This happens in general. We have one state with $m_{\max}$. Two states can have $m_{\max} - 1$, depending on whether we remove one unit from m' or from m''. Three states can have $m_{\max} - 2$, etc. Pictorially: [...] So in summary we haves:

$$|j'j'', m'm''\rangle\,, \quad m' = -j', ..., j'; \quad m'' = -j'', ..., j''\,. \tag{3.18}$$

$$|j'j''jm\rangle\,, \quad j = |j' - j''|, ..., j' + j''; \quad m = -j, ..., j\,. \tag{3.19}$$

Let's count number of states in the second case. Define $a = j' - j''$, $b = j' + j''$. We have:

$$\begin{aligned}\sum_{j=a}^{b}(2j+1) &= 2\sum_{j=a}^{b} j + \sum_{j=a}^{b} 1 = 2(\sum_{j=1}^{b} - \sum_{j=1}^{a-1}) + (b-a+1) \\ &= 2\frac{b(b+1)}{2} - 2\frac{(a-1)a}{2} + (b-a+1) \\ &= (j'+j'')(j'+j''+1) - (j'-j''-1)(j'-j'') + j'+j''-j'+j''+1 \\ &= 2j' + 2j'' + 4j'j'' + 1 = (2j'+1)(2j''+1)\,, \end{aligned} \tag{3.20}$$

which coindices precisely with the counting in the first basis.

By convention, all Clebsch-Gordan coefficients are real. Also, note that we can invert the relation between coefficients in one basis and in the other one:

$$|j'j'', m'm''\rangle = \sum_{jm} C_{j'j''}(jm, m'm'')|j'j''jm\rangle\,.$$

Spin operators

An operator of spin j is a set of $2j+1$ observables $\{O_j^m\}_{m=-j,\dots,j}$ fulfilling:

$$[J_3, O_j^m] = \hbar m O_j^m\,, \tag{3.21}$$

$$[J_\pm, O_j^m] = \hbar\sqrt{j(j+1) - m^2 \mp m}\, O_j^{m\pm1}\,; \tag{3.22}$$

or in other words $[\vec{J}, O_j^m] = \hbar \sum_{m'} \vec{J}^{(j)}_{m'm} O_j^{m'}$ where $\vec{J}^{(j)}_{m'm}$ is the spin-j representation of the angular momentum operators:

$$(J_3^{(j)})_{m'm} \equiv m\delta_{m'm}\,, (J_\pm)^{(j)})_{m'm} \equiv \sqrt{j(j+1) - m^2 \mp m}\,\delta_{m',m\pm1}\,. \tag{3.23}$$

Thus, scalar operators ($j = 0$) fulfill $[\vec{J}, O_0^0] = 0$. We say they're invariant under rotations. Vector operators have been defined as satisying $[J_i, V_j] = i\hbar\epsilon_{ijk}V_k$. Let's introduce spherical coordinates:

$$V^+ \equiv -\frac{V_1 + iV_2}{\sqrt{2}}\,, V^- \equiv \frac{V_1 - iV_2}{\sqrt{2}}\,, V^0 \equiv V_3\,. \tag{3.24}$$

Then:

$$[J_3, V^0] = [J_3, V_3] = i\hbar\epsilon_{33k}V_k = 0\,, \tag{3.25}$$

$$[J_3, V^+] = [J_3, -\frac{V_1}{\sqrt{2}}] + [J_3, -i\frac{V_2}{\sqrt{2}}] = -\frac{1}{\sqrt{2}}i\hbar\epsilon_{312}V_2 - \frac{i}{\sqrt{2}}i\hbar\epsilon_{321}V_1 = \hbar V^+\,, \tag{3.26}$$

$$[J_3, V^-] = -\hbar V^-\,. \tag{3.27}$$

So altogether we have $[J_3, V^m] = \hbar m V^m$. Moreover, we can find:

$$[J_\pm, V^m] = \hbar\sqrt{2 - m^2 \pm m}\, V^{m\pm1}\,.$$

So, in spherical components, a vector operator is a spin-1 operator. (They are one and the same thing really.)

Wigner-Eckart theorem

The Wigner-Eckart theorem restrict transition amplitudes involving spin-j operators. It reads:

$$\langle j''m''|O_j^m|j'm'\rangle = C_{jj'}(j''m'', mm')||O||\,,$$

where $||O||$ is certain quantity that does not depend on m, m', m''.

Let's prove this result, then we'll see implications. Consider arbitrary O_j^m of spin j, and let's build the state $O_j^m|j'm'\rangle$. We'll see that this state transform under rotations as any other state of composite system with j, m and j', m':

$$\begin{aligned} J_i O_j^m|j'm'\rangle &= [J_i, O_j^m]|j'm'\rangle + O_j^m J_i|j'm'\rangle \\ &= \hbar\sum_{m''}(J_i^{(j)})_{m''m}O_j^{m''}|j'm'\rangle + \hbar\sum_{m''}(J_i^{(j)})_{m''m'}O_j^m|j'm''\rangle\,. \end{aligned} \tag{3.28}$$

So $J_iO_j^m$ transforms under rotations like if it was a $|jj', mm'\rangle$. (Indeed, e.g. $J_3|jj', mm'\rangle = \hbar m|jj', mm'\rangle + \hbar m''|jj', mm'\rangle$.) This implies that it admits a decomposition in states of the form $|jj'j''m''\rangle$:

$$O_j^m|j'm'\rangle = \sum_{j''m''} C_{jj'}(j''m'', mm')|jj'j''m''\rangle\,. \tag{3.29}$$

Let's now compute what enters in the WE theorem, namely:

$$\begin{aligned} \langle j''m''|O_j^m|j'm'\rangle &= \sum_{j'''m'''} C_{jj'}(j'''m''', mm')\langle j''m''|jj'j'''m'''\rangle \\ &= C_{jj'}(j''m'', mm')\langle j''m''|jj'j''m''\rangle\,. \end{aligned} \tag{3.30}$$

where in the second equality we have used that, unless $j''' = j''$ and $m''' = m''$, the scalar product vanishes.

All that remains is proving that the braket is independent of m'' (obviously is independent of m and m'). For this, we use:

$$\begin{aligned} \langle jm+1\vec{\alpha}|jm+1\vec{\beta}\rangle &= \frac{1}{\hbar^2\sqrt{j(j+1)-m^2-m}}\langle jm+1\vec{\alpha}|J_+|jm\vec{\beta}\rangle \\ &= \frac{\hbar^2\sqrt{j(j+1)-(m+1)^2+(m+1)}}{\hbar^2\sqrt{j(j+1)-m^2-m}}\langle jm\vec{\alpha}|jm\vec{\beta}\rangle \\ &= \langle jm\vec{\alpha}|jm\vec{\beta}\rangle\,. \end{aligned} \tag{3.31}$$

So we can call $\langle j''m''|jj'j''m''\rangle \equiv ||O||$. This concludes the proof.

The most direct implication is that, up to an overall constant (independent of m, m' and m''), the following scalar products involving different vector operators are the same:

$$\langle j''m''|V^m|j'm'\rangle = C_{1j'}(j''m'', mm')||V||\,, \tag{3.32}$$

$$\langle j''m''|J^m|j'm'\rangle = C_{1j'}(j''m'', mm')||J|| \tag{3.33}$$

$$\Rightarrow \langle j''m''|V^m|j'm'\rangle = \frac{||V||}{||J||}\langle j''m''|J^m|j'm'\rangle\,. \tag{3.34}$$

This will be tremendously useful for computing transition amplitudes involving vectors operators, for which we'll simply replace the vector operator by angular momentum, which we know much better how to handle.

3.4 Internal and discrete symmetries

Inversions

These are transformations of the type $\vec{x} \to -\vec{x}$. Obviously they are not rotations ($\det(R) = -1$). They belong to $O(3)$ but not to $SO(3)$. There exists a unitarity operator $\mathcal{P}$ associated to parity.

On positions eigenstates, we have [CARE WITH INTERNAL PARITY!]:

$$\mathcal{P}|\vec{x}\rangle = |-\vec{x}\rangle \Rightarrow \vec{X}\mathcal{P}|\vec{x}\rangle = \vec{X}|-\vec{x}\rangle = -\vec{x}|-\vec{x}\rangle \Rightarrow \mathcal{P}^{-1}\vec{X}\mathcal{P}|\vec{x}\rangle = -\vec{x}\mathcal{P}^{-1}|-\vec{x}\rangle = -\vec{x}|\vec{x}\rangle$$

and so

$$\mathcal{P}^{-1}\vec{X}\mathcal{P} = -\vec{X}\,.$$

This holds for each particle position operator.

In what follows, we want to derive how parity acts on momentum, angular momentum and common Hamiltonian interactions.

For position, notice that:

$$\mathcal{P}|p\rangle = \mathcal{P}\int dx|x\rangle\langle x|p\rangle = \int dx\mathcal{P}|x\rangle\langle x|p\rangle = \int dx|-x\rangle\langle x|p\rangle \tag{3.1}$$

$$= \int dx|x\rangle\langle -x|p\rangle = \int dx|x\rangle\langle x|-p\rangle = |-p\rangle \Rightarrow \mathcal{P}^{-1}P\mathcal{P} = -\mathcal{P}\,. \tag{3.2}$$

In the last equality we've used that $\langle x|p\rangle = \exp(-ipx)$.

Now, for Hamiltonians of the form

$$H = \sum_n \frac{\vec{P}^2}{2m_n} + V(|\vec{X}_n - \vec{X}_m|$$

we have:

$$\mathcal{P}^{-1}H\mathcal{P} = \sum_n \frac{1}{2m_n}\mathcal{P}^{-1}\vec{P}\mathcal{P}\mathcal{P}^{-1}\vec{P}\mathcal{P} + V(|-\vec{X}_n + \vec{X}_m|) \tag{3.3}$$

$$= \sum_n \frac{1}{2m_n}(-\vec{P})(-\vec{P}) + V(|X_n - \vec{X}_m|) = H\,. \tag{3.4}$$

So this kind of Hamiltonian remains invariant. (Definitely, this is not the one of weak interactions, which involve sort of "square roots of momenta"...)

What about angular momentum?

$$(\mathcal{P}^{-1}\vec{L}\mathcal{P})_i = (\mathcal{P}^{-1}(\vec{X}\times\vec{P})\mathcal{P})_i = i\epsilon_{ijk}\mathcal{P}^{-1}X_jP_k\mathcal{P} \tag{3.5}$$

$$= i\epsilon_{ijk}\mathcal{P}^{-1}X_j\mathcal{P}^{-1}\mathcal{P}P_k\mathcal{P} = i\epsilon_{ijk}(-X_j)(-P_k) = L_i \Rightarrow [\vec{L},\mathcal{P}] = 0\,. \tag{3.6}$$

It can be also checked that $[\vec{S},\mathcal{P}] = [\vec{J},\mathcal{P}] = 0$. This implies that so, even in the presence of spin-orbit like effects ($\sim \vec{L}\cdot\vec{S}$), $[H,\mathcal{P}] = 0$.

Let's see how it acts on angular momentum eigenstates:

$$\mathcal{P}|lm\rangle = \mathcal{P}\int d\vec{x}|\vec{x}\rangle\langle\vec{x}|lm\rangle = \int dx|-\vec{x}\rangle R(|\vec{x}|)Y_l^m(\vec{x}) = \int d\vec{x}|\vec{x}\rangle R(|\vec{x}|)Y_l^m(-\vec{x}) \tag{3.7}$$

$$= \int d\vec{x}|\vec{x}\rangle R(|\vec{x}|)(-1)^lY_l^m(\vec{x}) \Rightarrow \mathcal{P}|lm\rangle = (-1)^l|lm\rangle\,.\,, \tag{3.8}$$

where $Y_l^m(\vec{x})$ are spherical harmonics. This has very important implications. Assume that the Hamiltonian of a Hydrogen-like atom includes subtle corrections so that all energy levels are non-degenerated (this must include spin-orbit but not only), but still $[H, \mathcal{P}] = 0$ and $[\vec{J}, H] = 0$ (though not necessarily orbital angular momenta or spin). It can be proven that, still, energy eigenstates of definite j have well defined ℓ!

To see why, let's proceed by reduction to the absurd. So assume that $|E\rangle$ is a linear combination of states with different ℓ, which by the way implies that $j = \ell + \frac{1}{2}$ or $j = \ell - \frac{1}{2}$:

$$|E\rangle = c_1 |j + \frac{1}{2}\ m\rangle + c_2 |j - \frac{1}{2}\ m\rangle \,.$$

Now note that:

$$H\mathcal{P}|E\rangle = \mathcal{P}H|E\rangle = E\mathcal{P}|E\rangle$$

so, given that energy levels are not degenerated, $\mathcal{P}|E\rangle$ is also an eigenstate with energy E, namely $\mathcal{P}|E\rangle \propto |E\rangle$.

So:

$$\mathcal{P}|E\rangle = c_1 \mathcal{P}|j - \frac{1}{2}\ m\rangle + c_2 \mathcal{P}|j + \frac{1}{2}\ m\rangle = c_1 (-1)^{j+\frac{1}{2}} |j + \frac{1}{2}\ m\rangle + c_2 (-1)^{j-\frac{1}{2}} |j - \frac{1}{2}\ m\rangle \,,$$

but this has necessarily a relative sign! So it can not be $\propto |E\rangle$. So the assumption is wrong and therefore ℓ is necessarily well defined.

Let's come back to how parity acts on position eigenstates. What we really have in practice is:

$$\mathcal{P}|x\rangle = \eta |-\vec{x}\rangle \,,$$

because state is defined up to phase. Necessarily:

$$\eta^2 = 1 \Rightarrow \eta = \pm 1 \,.$$

It can be though as an internal parity (or the eigenvalue of certain internal symmetry).

3.4.1 Time reversal

In classical mechanics, time reversal means replacing $t \to -t$. In quantum mechanics, the state $\psi(x,t)$ evolves according to Schrödinger's equation:

$$i\hbar \frac{\partial}{\partial t} \psi(x,t) = H\psi(x,t). \tag{3.9}$$

Under $t \to -t$, we want the time-reversed wave function $\psi_T(x,t)$ to satisfy the same equation:

$$i\hbar \frac{\partial}{\partial t} \psi_T(x,t) = H\psi_T(x,t). \tag{3.10}$$

If we naively define $\psi_T(x,t) = T\psi(x,-t)$ with a *linear and unitary* T, then inserting this into Eq. (3.9) gives

$$-i\hbar \frac{\partial}{\partial t} \psi_T(x,t) = H\psi_T(x,t), \tag{3.11}$$

which has the wrong sign in front of i.

To restore Schrödinger's equation, T must send $i \to -i$. However, i is not an operator but a scalar, so the only way to achieve this is to define T such that it *complex-conjugates*

scalars. Therefore T must be **antilinear**, not linear and so, according to Wigner's theorem, also **anti-unitary**.

Let the wave function in position representation be $\psi(x,t)$. Time reversal acts as:

$$(T\psi)(x,t) = \psi^*(x,-t), \tag{3.12}$$

i.e. it reverses time and complex-conjugates the amplitudes. It can be trivially checked that this is indeed the simplest anti-linear and antiunitary operation.

At $t=0$,

$$(T\psi)(x) = \psi^*(x). \tag{3.13}$$

Now, let's see how T acts on different operators, starting with X.

Since position acts multiplicatively,

$$(TXT^{-1}\psi)(x) = T(x\,\psi^*(x)) = x\,\psi(x), \tag{3.14}$$

so

$$\boxed{TXT^{-1} = X.} \tag{3.15}$$

Momentum in position space is $P = -i\hbar\partial_x$:

$$(TPT^{-1}\psi)(x) = T\big(-i\hbar\,\partial_x\psi^*(x)\big) = +i\hbar\,\partial_x\psi(x) = (-P\psi)(x), \tag{3.16}$$

hence

$$\boxed{TPT^{-1} = -P.} \tag{3.17}$$

For the orbital angular momentum, $L = XP - PX$:

$$TLT^{-1} = (TXT^{-1})(TPT^{-1}) - (TPT^{-1})(TXT^{-1}) = X(-P) - (-P)X = -L. \tag{3.18}$$

Thus,

$$\boxed{TLT^{-1} = -L.} \tag{3.19}$$

This works for any other angular momentum, like spin.

For the free Hamiltonian, $H = \frac{P^2}{2m}$,

$$THT^{-1} = \frac{(-P)^2}{2m} = H, \tag{3.20}$$

so the free Hamiltonian is *time-reversal invariant*. Most fundamental known Hamiltonians are, with the exception of the one of week interactions [there's also debate about strong interactions, related to the so-called strong-CP problem.]

Example 5. Kramers Degeneracy

Assume H is time-reversal invariant. Assume also that $T^2 = -1$. This happens for example in systems with an odd number of spin-1/2 fermions [2]

If $|\psi\rangle$ is an eigenstate of H,

$$H|\psi\rangle = E|\psi\rangle,$$

then

$$H(T|\psi\rangle) = T(H|\psi\rangle) = E(T|\psi\rangle),$$

[2]Indeed, since simply as any other angular momentum, $TS_iT^{-1} = -S_i$, it can be checked that in a 2-state system T is simply $T = i\sigma_y K$ where K stands for complex conjugation. Therefore, $T^2 = -\sigma_y^2 = -1$.

so $T|\psi\rangle$ is another eigenstate with the same energy E.

Now, these two vectors do not represent the same state, because they are orthogonal. Indeed, define $|\phi\rangle \equiv= T|\psi\rangle$. Then, by anti-unitarity:

$$\langle\psi|T^\dagger T|\phi\rangle = \langle\psi|\phi\rangle^* \tag{3.21}$$

This implies:

$$\langle\psi|T^\dagger T^2|\psi\rangle = \langle\psi|T|\psi\rangle^* \tag{3.22}$$

but it is also true, because $T^2 = -1$, that the LHS gives $-\langle\psi|T^\dagger|\psi\rangle$ which is the same (according to scalar-product rules and the definition of hermitian) as $-\langle\psi|T|\psi\rangle$. So we get that, for $z = \langle\psi|T|\pi\rangle$, $z^* = -z$. This can only be satisfied if $z = 0$:

$$\boxed{\langle\psi|T|\psi\rangle = 0.} \tag{3.23}$$

Therefore $|\psi\rangle$ and $T|\psi\rangle$ are orthogonal but degenerate:

$$H|\psi\rangle = E|\psi\rangle, \qquad H(T|\psi\rangle) = E(T|\psi\rangle).$$

The prime example of Kramer's degeneracy is the Hydrogen-like atom degenerated in m (third component of total angular momentum). This is lifted in the presence of a magnetic field $\vec{B}$ that introduces an interaction of the sort $\sim \vec{B}\cdot\vec{L}$ because angular momentum is odd under the action of T but B remains invariant. We will see this when discussing the Zeeman effect. [This could be also explained using the fact that $\vec{B}$ breaks rotational invariance.]

3.5 Exercises

Exercise 3.5.1 *A particle in 1D has normalized wavefunction*

$$\psi(x) = \sqrt{\frac{2}{L}}\sin\frac{\pi x}{L}\,, \quad 0 < x < L\,.$$

Compute the expectation values $\langle P\rangle_\psi$ and $\langle P\rangle_{\psi_a}$ where $\psi_a(x) = \psi(x-a)$. Explain the result using symmetry.

Solution. With $P = -i\hbar\,\partial_x$ and ψ real,

$$\langle P\rangle_\psi = \int_0^L \psi(x)\,(-i\hbar\,\partial_x\psi(x))\,dx = -\frac{i\hbar}{2}\int_0^L \partial_x\big(\psi^2(x)\big)\,dx = -\frac{i\hbar}{2}\Big[\psi^2(x)\Big]_0^L = 0,$$

since $\psi(0) = \psi(L) = 0$.

Now consider the translated state $\psi_a(x) = \psi(x-a)$. In operator language, this is obtained via the translation operator

$$T(a) = e^{-iaP/\hbar}, \qquad |\psi_a\rangle = T(a)|\psi\rangle.$$

The expectation value of momentum in the translated state is

$$\langle P\rangle_{\psi_a} = \langle\psi_a|P|\psi_a\rangle = \langle\psi|T^\dagger(a)\,P\,T(a)|\psi\rangle.$$

Because P is the generator of translations, it commutes with its exponential:

$$T^\dagger(a)\, P\, T(a) = P.$$

Hence,

$$\langle P\rangle_{\psi_a} = \langle\psi|P|\psi\rangle = \langle P\rangle_\psi.$$

Since we already found $\langle P\rangle_\psi = 0$, it follows that

$$\boxed{\langle P\rangle_{\psi_a} = 0 \quad \forall\, a.}$$

Exercise 3.5.2 *The observable A of certain physical system has non-degenerated eigenvalues of eigenvectors $|a_i\rangle$, $i = 1, 2$. Let K be a linear operator defined by*

$$K|a_1\rangle = |a_2\rangle\,, \quad K|a_2\rangle = |a_1\rangle\,.$$

The Hamiltonian of the system commutes with K, and the eigenenergies are non-degenerated.

(a) Does K represent an observable? Does it represent a symmetry transformation? If so, what is the smallest symmetry group that contains this transformation?

(b) Write the matrix of the Hamiltonian in the basis of eigenstates of A.

(c) The observable A is measured at $t = 0$. What is the probability of obtaining the same value if A is again measured at a later tiem?

Exercise 3.5.3 *Let $\vec{A}$ and $\vec{B}$ be vector operators. Prove that $\vec{A}\times\vec{B}$ is also a vector operator.*

Solution. By definition,

$$C_i = (\vec{A}\times\vec{B})_i = \epsilon_{ijk}A_jB_k. \tag{3.1}$$

Then,

$$[J_l, C_i] = [J_l, \epsilon_{ijk}A_jB_k] \tag{3.2}$$

$$= \epsilon_{ijk}\big([J_l, A_j]B_k + A_j[J_l, B_k]\big), \tag{3.3}$$

using the Leibniz rule for commutators.

Since $\vec{A}$ and $\vec{B}$ are vector operators,

$$[J_l, A_j] = i\hbar\,\epsilon_{ljm}A_m, \qquad [J_l, B_k] = i\hbar\,\epsilon_{lkn}B_n. \tag{3.4}$$

Substituting these relations gives

$$[J_l, C_i] = i\hbar\,\epsilon_{ijk}\left(\epsilon_{ljm}A_mB_k + \epsilon_{lkn}A_jB_n\right). \tag{3.5}$$

We now simplify each term using the identity

$$\epsilon_{ijk}\epsilon_{ljm} = \delta_{il}\delta_{km} - \delta_{im}\delta_{kl}. \tag{3.6}$$

Applying this identity to both terms, we find after straightforward algebra:

$$[J_l, C_i] = i\hbar\,\epsilon_{lim} C_m. \tag{3.7}$$

Exercise 3.5.4 *The Hamiltonian of a particle of mass m and spin $\vec{S}$ in a magnetic field $\vec{B} = B\hat{z}$ is given by*

$$H = \frac{\vec{P}^2}{2m} - \mu B S_3\,,$$

where μ is constant. Derive the equations for the time evolution of the expectation values of the three components of $\vec{S}$.

Solution. We'll work in Heisenberg's picture:

$$\begin{aligned}\dot{S}_i &= \frac{i}{\hbar}[H, S_i] = \frac{i}{\hbar}[\frac{\vec{P}^2}{2m}, S_i] - i\frac{\mu}{\hbar}B[S_3, S_i] \\ &= \mu B\epsilon 3ij S_j\,,\end{aligned} \tag{3.8}$$

from where $\dot{S}_1 = \mu B S_2$, $\dot{S}_2 = -\mu B S_1$ and $\dot{S}_3 = 0$. Taking the time derivative:

$$\ddot{S}_1 = \mu B\dot{S}_2 = -\mu^2 B^2 S_1 \tag{3.9}$$

$$\ddot{S}_2 = -\mu B\dot{S}_1 = \mu^2 B^2 S_2\,. \tag{3.10}$$

and so

$$\langle S_1(t)\rangle = \langle S_1(0)\rangle \cos\mu BT + \langle S_2(0)\rangle \sin\mu Bt\,, \tag{3.11}$$

$$\langle S_2(t)\rangle = \langle S_2(0)\rangle \cos\mu BT + \langle S_1(0)\rangle \sin\mu Bt\,, \tag{3.12}$$

$$\langle S_3(t)\rangle = \langle S_3(0)\rangle\,. \tag{3.13}$$

Exercise 3.5.5 *Consider an electron with orbital angular momentum $\ell = 2$. Without using the table of Clebsh-Gordan coefficients, build the states with total angular momentum $j = 5/2$ and $m = 5/2, 3/2$ as linear combinations of states with definite L_3 and S_3. Find likewise the state with $j = m = 3/2$.*

Solution. We have $l = 2, s = 1/2$. The maximum j is $j = 2 + 1/2 = 5/2$. The maximum m is also $m = 5/2$. We have then:

$$|2\tfrac{1}{2}\tfrac{5}{2}\tfrac{5}{2}\rangle = |2\tfrac{1}{2}, 2\tfrac{1}{2}\rangle\,.$$

Now, to build the state $|2\frac{1}{2}\frac{5}{2}\frac{3}{2}\rangle$, we use that

$$(J_1 + iJ_2)|lsjm\rangle = \hbar\sqrt{j(j+1) - m^2 \mp m}\,|lsjm-1\rangle$$

implying that

$$\begin{aligned}|2\tfrac{1}{2}\tfrac{5}{2}\tfrac{3}{2}\rangle &= \frac{1}{\hbar}\frac{1}{\sqrt{5/2(5/2+1) + (5/2)^2 + 5/2}}(J_1 - iJ_2)|2\tfrac{1}{2}\tfrac{5}{2}\tfrac{5}{2}\rangle \\ &= \frac{1}{\sqrt{5}\hbar}(L_1 - iL_2 + S_1 - iS_2)|2\tfrac{1}{2}, 2\tfrac{1}{2}\rangle \\ &= \frac{2}{\sqrt{5}}|2\tfrac{1}{2}, 1\tfrac{1}{2}\rangle + \frac{1}{\sqrt{5}}|2\tfrac{1}{2}, 2 - \tfrac{1}{2}\rangle\,.\end{aligned} \tag{3.14}$$

THe state with $j = m = 3/2$ can be only a linear combination of states with $m_l = 1, m_s = 1/2$ and $m_l = 2, m_s = 1/2$. Any other combination of $m_l = -2, -1, 0, 1, 2$ and $m_s = \pm 1/2$ gives $m_l + m_s \neq 3/2$.

So, $|2\frac{1}{2}\frac{3}{2}\frac{3}{2}\rangle = \alpha_1|2\frac{1}{2}, 1\frac{1}{2}\rangle + \alpha_2|2\frac{1}{2}, 2-\frac{1}{2}\rangle$, but since it has $j = 3/2$ it must be orthogonal to $|2\frac{1}{2}\frac{5}{2}\frac{3}{2}\rangle$ which has $j = 5/2$. The only solution (up to a phase) is:

$$|2\frac{1}{2}\frac{5}{2}\frac{3}{2}\rangle = -\frac{1}{\sqrt{5}}|2\frac{1}{2}, 2-\frac{1}{2}\rangle + \frac{2}{\sqrt{5}}|2\frac{1}{2}, 1\frac{1}{2}\rangle\,.$$

Exercise 3.5.6 *Consider an electron with $\ell = 0$ in atom whose nucleus has spin $I = 3/2$. Write the states of the atom with third component of total angular momentum $m = 1$ and arbitary j as linear combinations of states with definite values of S_3 of the electron and the nucleus.*

Solution. We have $l = 0$, $s = 1/2$ and $I = 3/2$. So the possible values of j are $j = 1, 2$.

The two of them have states with $m = 1$. Let's start with $j = 2, m = 1$. Simply reading the table of Clebsh-Gordan coefficients:

$$|\frac{1}{2}\frac{3}{2}21\rangle = \frac{3}{2}|\frac{1}{2}\frac{3}{2}, \frac{1}{2}\frac{1}{2}\rangle + \frac{1}{2}|\frac{1}{2}\frac{3}{2}, -\frac{1}{2}\frac{3}{2}\rangle\,.$$

Likewise, for $j = 1, m = 1$, we have:

$$|\frac{1}{2}\frac{3}{2}11\rangle = \frac{3}{2}|\frac{1}{2}\frac{3}{2}, -\frac{1}{2}\frac{3}{2}\rangle - \frac{1}{2}|\frac{1}{2}\frac{3}{2}, \frac{1}{2}\frac{1}{2}\rangle$$

which is simply orthogonal to the first.

Exercise 3.5.7 *Consider a particle of spin $s = 1$. For which state it is certain that a measurement of the spin in an arbitrary direction, namely of $\hat{n} \cdot \vec{S}$ with*

$$\hat{n} = \sin\theta(\hat{x}\cos\phi + \hat{y}\sin\phi) + \cos\theta\hat{z}\,,$$

is precisely $\hbar$? And for which it is zero?

Exercise 3.5.8 *A system of two particles with spins $s_1 = 3/2$ and $s_2 = 1/2$ is described by the Hamiltonian*

$$H = g\vec{S}_1 \cdot \vec{S}_2\,,$$

where g is a constant. At $t = 0$, the system in is an eigenstate of S_{1z} and S_{2z} with eigenvalues $3\hbar/2$ and $\hbar/2$, respectively. Find the state of the system at $t \geq 0$. What is the probability of obtaining $3\hbar/2$ and $-\hbar/2$ in a simultaneous measurement of S_{1z} and S_{2z}? How do things change if the state at $t = 0$ is an eigenstate of S_{1z} and S_{2z} with both eigenvalues $\hbar/2$?

Exercise 3.5.9 *A particle of spin $s = 3/2$ decays into a nucleon ($\eta_N = +1$ and a pion ($\eta_\pi = -1$). Show that angular distribution of the final state can be used to determine the parity of the decaying particle.*

Nucleons have $s = 1/2$ while pions have $s = 0$. So, from angular momentum conservation (in the initial frame the particle is at rest, so $\ell = 0$ and $j = s = 3/2$), $\ell = 3/2 - 1/2, 3/2 + 1/2 = 1, 2$. Assuming that parity is conserved in the decay:

$$\eta = (-1)^{\ell}\eta_N\eta_\pi = (-1)^{\ell+1} .$$

Angular momentum distribution measurements can determine whether $\ell = 1$ or $\ell = 2$, from where it follows $\eta = 1$ or $\eta = -1$.

Chapter 4

Approximate Methods

4.1 Perturbation theory

There are very few exactly solvable systems: free particle, Coulomb potential, harmonic oscillator.

In general most system can be only solved approximately (e.g. two-electron atoms). In practice, we even want to have approximate solutions only, because the exact solutoin might be not very enlightening.

Perturbation theory is probably the best approach to approximate solutions. The idea is consider the limit of exactly solvable + small perturbation.

Time-independent perturbation theory

Let's consider first approximations to energy eigenvalues (which in general are hard to compute exactly). Assume we have:

$$H_0|a\rangle = E_a|a\rangle\,,$$

with $\langle a|b\rangle = \delta_{ab}$.

This is the Hamiltonian we assume we know how to solve exactly. It could be the Coulomb potential Hamiltonian $H_0 \sim K - \alpha/r$. Let's know have

$$H = H_0 + \delta H$$

where δH is controled by a small parameter $\epsilon \ll 1$. It could for example be $\delta H = \epsilon\alpha'/r^2$.

Then, we expect the eigenstates of the full Hamiltonian to be

$$|a\rangle + \epsilon|\delta a\rangle + \mathcal{O}(\epsilon^2)$$

with

$$E = E_a + \epsilon\delta E_a + \mathcal{O}(\epsilon^2)\,.$$

This means:

$$(H_0 + \delta H)(|a\rangle + |\delta a\rangle) = (E_a + \delta E_a)(|a\rangle + |\delta a\rangle) \tag{4.1}$$

$$\Rightarrow H_0|a\rangle + \delta H|a\rangle + H_0|\delta a\rangle + \mathcal{O}(\epsilon^2) = E_a|a\rangle + E_a|\delta a\rangle + \delta E_a|a\rangle + \mathcal{O}(\epsilon^2) \tag{4.2}$$

$$\Rightarrow \delta H|a\rangle + H_0|\delta a\rangle = \delta E_a|a\rangle + E_a|\delta a\rangle\,. \tag{4.3}$$

Let's take the scalar product of this expression with $|a\rangle$:

$$\langle a|\delta H|a\rangle + \langle a|H_0|\delta a\rangle = \delta E_a\langle a|a\rangle + E_a\langle a|\delta a\rangle \tag{4.4}$$

$$\Rightarrow \langle a|\delta H|a\rangle + E_a\langle a|\delta a\rangle \qquad = \delta E_a\langle a|a\rangle + E_a\langle a|\delta a\rangle \tag{4.5}$$

$$\Rightarrow \langle a|\delta H|a\rangle = \delta E_a\,. \tag{4.6}$$

In the first implication we have applied H_0 on the bra.

This result allows us to compute the energy shift to first approximation. Let's also see how the state vector changes under perturbation. To this aim we now take the scalar product with $|b\rangle \neq |a\rangle$:

$$\langle b|\delta H|a\rangle + \langle b|H_0|\delta a\rangle = \delta E_a\langle b|a\rangle + E_a\langle b|\delta a\rangle = E_a\langle b|\delta a\rangle$$

which implies (provided $E_a \neq E_b$):

$$\langle b|\delta H|a\rangle = (E_a - E_b)\langle b|\delta a\rangle \Rightarrow \langle b|\delta a\rangle = \frac{\langle b|\delta H|a\rangle}{E_a - E_b}$$

Now, notice that

$$|\delta a\rangle = \sum_b |b\rangle\langle b|\delta a\rangle = \sum_{b\neq a} |b\rangle \frac{\langle b|\delta H|a\rangle}{E_a - E_b} + \langle a|\delta a\rangle|a\rangle = \sum_{b\neq a} |b\rangle \frac{\langle b|\delta H|a\rangle}{E_a - E_b}$$

because the last term vanishes. To see why, take the scalar product of $|a\rangle + \epsilon|\delta a\rangle$ with itself, which gives:

$$1 = 1 + \epsilon\langle a|\delta a\rangle + \epsilon\langle \delta a|a\rangle + \mathcal{O}(\epsilon^2)\,.$$

Now, this implies:

$$\mathrm{Re}\langle \delta a|a\rangle = 0 \Rightarrow \langle \delta a|a\rangle = 0\,,$$

where in the last implication we have used that we can always make a phase transformation on $|a\rangle$ to make the scalar product real.

Let's notice now that perturbation theory breaks if there's some state $|b\rangle$ with $E_b = E_a$, since the perturbation produces a infinite modification of the state vector. Unless, $\langle b|\delta H|a\rangle = 0$. We'll see one example of how to fix it (this has been studied in Quantum Physics); for now we'll apply perturbation theory where it works.

One obvious case is the spin-orbit interaction,

$$\delta H = \mu \vec{L}\cdot\vec{S}\,.$$

If we take H_0 to be the usual Coulomb Hamiltonian, then the states are $|nljm\rangle$, and they fulfill $\langle n'l'j'm'|nljm\rangle = 0$ if $n \equiv n'$ or any other quantum number differs. Moreover,

$$\langle n'l'j'm'|\delta H|nljm\rangle = \frac{\mu}{2}\langle n'l'j'm'|\vec{J}^2 - \vec{L}^2 - \vec{S}^2|nljm\rangle \tag{4.7}$$

$$= \frac{\mu\hbar^2}{2}(j(j+1) - l(l+1) - s(s+1))\langle n'l'j'm'|nljm\rangle\,. \tag{4.8}$$

This implies also that, although energy levels shift, the states remain the same.

Zeeman effect

This is the Hydrogen-like atom in the presence of a magnetic field, which produces a perturbation

$$\delta H = \frac{e}{2m_e c}\vec{B}\cdot(\vec{L}+g_e\vec{S})\,.$$

(By the way, $g_e = 2.00231930436(1)$ is astonishing.) We consider that H_0 contains the Coulomb potential (which has energy levels degenerated in j, l, m) but also any other interactions that break the degeneracy in j, l. Whatever these interactions are, must be significantly smaller then the coulomb (so that we use perturbation theory with the usual Hamiltonian), but significantly larger than the magnetic field effect, to use perturbation theory with those states as basic ones.

As we have seen before, the states in the presence of spin-orbit coupling are the same, but now they degeneracy in l and j is broken. Let's compute the shift to the energy (which itself is a double shift to the original Coulomb energy). To on the fly see that perturbation theory works, let compute the more general amplitude

$$\langle nljm'|\vec{L}+g_e\vec{S}|nljm\rangle = g_{njl}\langle nljm'|\vec{J}|nljm\rangle \tag{4.9}$$

where we have used the Wigner-Eckart theorem (g does not depend on m, m' precisely because is a ratio of reduced matrix elements). We call this the Landé g-factor.

This way, computing the matrix element is trivial once we go to a reference system in which $\vec{B} = B\hat{z}$, but we still need to compute g_{nlj}. To this aim:

$$\vec{J}^2 J_i|nljm\rangle = J_i\vec{J}^2|nljm\rangle = \hbar j(j+1)J_i|nljm\rangle \Rightarrow J_i|nljm\rangle = \sum_{m''} c_{m''}|nljm''\rangle\,. \tag{4.10}$$

In the implication we have used that $J_i|nljm\rangle$ is an eigenstate of $\vec{J}^2$ and so a linear combination of all possible one (which differ only by m''). So, we also have:

$$\langle nljm'|(L_j+g_eS_j)J_i|nljm\rangle = \sum_{m''} c_{m''}\langle nljm'|(L_j+g_eS_j)|nljm''\rangle \tag{4.11}$$

$$= g_{nlj}\sum_{m''} c''_m\langle nljm'|J_j|nljm''\rangle \tag{4.12}$$

$$= g_{nlj}\langle nljm'|J_jJ_i|nljm\rangle\,. \tag{4.13}$$

Let's now fix $j = i$, and sum over i:

$$\sum_i\langle nljm|(L_i+g_eS_i)J_i|nljm\rangle = g_{nlj}\sum_i\langle nljm|J_iJ_i|nljm\rangle \tag{4.14}$$

$$= g_{nlj}\hbar^2 j(j+1)\,. \tag{4.15}$$

Now note that $\vec{S} = \vec{J}-\vec{L}$ and so $\vec{S}^2 = \vec{J}^2+\vec{L}^2-2\vec{L}\cdot\vec{J}$. Hence:

$$\sum_i L_iJ_i|nljm\rangle = \frac{1}{2}(-\vec{S}^2+\vec{L}^2+\vec{J}^2)|nljm\rangle \tag{4.16}$$

$$= \frac{\hbar^2}{2}\left[\frac{-3}{4}+l(l+1)+j(j+1)\right]|nljm\rangle \tag{4.17}$$

Proceeding similarly, we find:

$$\sum S_i J_i |nljm\rangle = \frac{1}{2}\Big[-\vec{L}^2 + \vec{S}^2 + \vec{J}^2]|nljm\rangle = \frac{\hbar}{2}\Big[-l(l+1) + \frac{3}{4} + j(j+1)\Big]|nljm\rangle \,. \tag{4.18}$$

Altogether:

$$\frac{1}{2}[-\frac{3}{4} + l(l+1) + j(j+1)] + \frac{g_e}{2}[-l(l+1) + \frac{3}{4} + j(j+1)] = j(j+1)g_{nlj} \tag{4.19}$$

$$\Rightarrow g_{nlj} = 1 + (g_e - 1)\left[\frac{j(j+1) - l(l+1) + 3/4}{2j(j+1)}\right]. \tag{4.20}$$

Now that we have $g_{jl} \equiv g_{nlj}$ (just saw it does not depend on n), we can simply come back to Wigner-Eckart theorem:

$$\langle nljm'|\delta H|nljm\rangle = \frac{e}{2m_e c} g_{jl} \langle nljm'|\vec{B}\cdot\vec{J}|nljm\rangle = \frac{e\hbar g_{jl} B}{2m_e c} m\delta_{mm'} \tag{4.21}$$

So the braket with the perturbation between two different states with same energy vanishes, so we can use it for computing energy shifts:

$$\delta E_{nljm} = \frac{e\hbar g_{jl} B}{2m_e c} m \,. \tag{4.22}$$

This breaks completely the degeneracy. (The states are the same though, and ℓ is well defined!)

Time-dependent perturbation theory

Let us consider

$$H(t) = H_0 + \delta H(t) \,.$$

We assume that the spectrum of H_0 is known, so

$$H_0|E_n\rangle = E_n|E_n\rangle \,,$$

with $\langle E_n|E_m\rangle = \delta_{nm}$.

For any $t \in \mathbb{R}$, $|\psi(t)\rangle \in \mathcal{H}$, so we can decompose in the basis of eigenstates of H_0, namely:

$$|\psi(t)\rangle = \sum_n \tilde{c}_n(t)|E_n\rangle = \sum_n c_n(t) e^{\frac{-iE_n t}{\hbar}}|E_n\rangle \,, \tag{4.23}$$

having defined $c_n(t) \equiv \tilde{c}_n(t) e^{\frac{iE_n t}{\hbar}}$.

Likewise, we can expand

$$\delta H(t)|E_n\rangle = \sum_m |E_m\rangle\langle E_m|\delta H(t)|E_n\rangle \equiv \sum_m \delta H_{mn}(t)|E_m\rangle \,.$$

Altogether, the full Schröringer equation reads:

$$i\hbar\frac{d|\psi(t)\rangle}{dt} = H(t)|\psi(t)\rangle \Rightarrow \tag{4.24}$$

$$\sum_n \left[i\hbar\frac{dc_n(t)}{dt} + E_n c_n(t)\right] e^{\frac{-iE_n t}{\hbar}}|E_n\rangle = \sum_n c_n(t)\left[E_n|E_n\rangle + \sum_m \delta H_{mn}(t)|E_m\rangle\right] e^{\frac{-iE_n t}{\hbar}} \,. \tag{4.25}$$

Canceling the terms with E_n, renaiming $n \leftrightarrow m$ in the double sum, and because $|E_n\rangle$ expand a basis, we get:

$$i\hbar\frac{dc_n(t)}{dt} = \sum_m \delta H_{nm}(t)c_m(t)e^{i\frac{(E_n-E_m)t}{\hbar}} . \tag{4.26}$$

A diffrent way of writting this is

$$i\hbar\dot{\mathbf{c}}(t) = H_I(t)\mathbf{c}(t) .$$

This can be solved upon integrating between t_0 and t on each side, but we'll do it in operator form for clarity. From here we can define the evolution opertor $U_I(t,t_0)$ such that $\mathbf{c}(t) = U_I(t,t_0)\mathbf{c}(t_0)$ with $U_I(t_0,t_0) = 1$. Therefore:

$$i\hbar\dot{U}_I(t,t_0) = H_{\text{eff}}(t)U_I(t,t_0) .$$

(In here we have taken that two linear operators that are the same when acting on any $c(t_0)$ (arbitrary vector) are equal. This can be trivially solved, upon integrating between t_0 and t on each side:

$$U_I(t,t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t} dt' H_I(t')U(t',t_0) .$$

Let's solve this to first order, we simply take $U = 1$. Then:

$$U_I(t,t_0) \sim 1 - \frac{i}{\hbar}\int_{t_0}^{t} dt_1 H_I(t_1) .$$

To next order, we substitute the first approximation of U in the ingrand:

$$U_I(t,t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t} dt_2 H_I(t_2)\left[1 - \frac{i}{\hbar}\int_{t_0}^{t_2} dt_1 H_I(t_1)\right]$$

which gives:

$$U_I(t,t_0) \sim 1 - \frac{i}{\hbar}\int_{t_0}^{t} dt_2 H_I(t_2) - \frac{1}{\hbar^2}\int_{t_0}^{t}\int_{t_0}^{t_2} dt_2 dt_1 H_I(t_2)H_I(t_1) .$$

This can be iterated to all orders, obtaining:

$$U_I(t,t_0) = \mathcal{T}\exp -\frac{i}{\hbar}\int_{t_0}^{t} dt' H_I(t')$$

where $\mathcal{T}$ means time ordering [DEFINE].

As an example, let's consider monochromatic perturbations, defined by

$$\delta H(t) = -Ue^{-i\omega t} - U^\dagger e^{i\omega t}$$

with $\omega > 0$. This model an incident (electromagnetic) wave. Note both terms in the perturbation, otherwise it is not Hermitian.

We have:

$$c_n(t) = c_n(0) + \sum_m U_{nm} c_m(0) \frac{1}{E_n - E_m - \hbar\omega} \left[e^{i\frac{(E_n - E_m - \hbar\omega)t}{\hbar}} - 1 \right] \tag{4.27}$$

$$+ \sum_m U^*_{mn} c_m(0) \frac{1}{E_n - E_m + \hbar\omega} \left[e^{i\frac{(E_n - E_m + \hbar\omega)t}{\hbar}} - 1 \right]. \tag{4.28}$$

Let us focus in the case $c_n(0)0$ for all $n \neq 1$ (and so $c_1(t) = 1$). Physically, this implies that the unperturbed system is in the ground state. Our goal is computing the probability of exiting into a different one. We have:

$$c_n(t) = U_{n1} \left[\frac{e^{i\frac{(E_n - E_1 - \hbar\omega)t}{\hbar}} - 1}{E_n - E_1 - \hbar\omega} \right] + U^*_{1n} \left[\frac{e^{i\frac{(E_n - E_1 - \hbar\omega)t}{\hbar}} - 1}{E_n - E_1 + \hbar\omega} \right] \tag{4.29}$$

which obviously vanishes at $t = 0$. We can distinguish two important limits here, the **absortion** region ($E_n \sim E_1 + \hbar\omega$) and the **stimulated emission** region ($E_n \sim E_1 - \hbar\omega$). In each limit, one of the terms dominates. Thus, e.g. in the absortion region, we have:

$$c_n(t) \to U_{n1} \left[\frac{e^{i\frac{(E_n - E_1 - \hbar\omega)t}{\hbar}} - 1}{E_n - E_1 - \hbar\omega} \right] \tag{4.30}$$

and so the probability of the system of getting excited after certain time t is:

$$|\langle E_n|\phi(t)\rangle|^2 = |c_n(t)|^2 \sim 4|U_{n1}|^2 \frac{1}{(E_n - E_1 - \hbar\omega)^2} \sin^2 \frac{(E_n - E_1 - \hbar\omega)t}{2\hbar} \tag{4.31}$$

which can be approximated at large t (and because $E_n - E_1 - \hbar\omega \to 0$) by a Dirac delta function:

$$|c_n(t)|^2 = 4|U_{n1}|^2 \frac{\pi t}{2\hbar} \delta(E_1 + \hbar\omega - E_n)\,. \tag{4.32}$$

The transition rate, defined as the probability of excitation per unit time, becomes:

$$\Gamma(1 \to n) \equiv \frac{|c_n(t)|^2}{t} = \frac{2\pi}{\hbar} |U_{n1}|^2 \delta(E_1 + \hbar\omega - E_n)\,. \tag{4.33}$$

This is known as **Fermi's Golden rule**.

Exercise 4.1.1 ■ *Consider a one-dimensional harmonic oscillator of frequency ω, mass m and electric charge q. At $t = 0$, the oscillator is at the ground state. Then, a small constant electric field $V(x) = -qEx$ is applied during a time τ, after which it is removed and the system remains unperturbed for a time T. Afterwards, again, the constant electric field is switched on during a time τ.*

(a) Compute, to first order in perturbation theory, the probability that the system is excited at the end of the process.

(b) Does this probability depend on the time T during which the system is not perturbed? Why?

□

4.2 Scattering theory