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Quantum Mechanics II

2020-21 class

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* DCU

Quantum Mechanics II, 2020-21 class

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1 Prelude

The lectures go through concepts, methods and applications covering this physical theory known under the general term *Quantum Mechanics* (QM). It can be argued that Quantum mechanics was developed as the first physical theory capable to provide quantitative description of natural events occurring in systems of the atomic scale. [1] Due to technological advances near the end of the 19th century a wealth of spectroscopic data were available, requiring understanding; with the most notable case being the *black body radiation* distribution spectrum. Quantum mechanics was mainly developed the years following Max-Planck's breakthrough assumption of discrete energies of the harmonic oscillator problem in his treatment of black-body radiation (1900) and Einstein's hypothesis of light propagation in bunches (1905). QM theory had firmly established until the year 1930 (collectively known as 'Copenhagen interpretation') by Niels Bohr, Heisenberg, Born, Dirac, Kramer, Jordan et al, with the core principles already concluded around the years 1925-27 *et al* [1]. The approach of this School has succeed to incorporate in its principles (often called a matrix-mechanics approach) and the alternative and completely equivalent, *wave-mechanics* formulation of Erwin Schrödinger in 1926 [2].

Around the same time the QM's physical principles were put on firm mathematical basis using the language of Hilbert vector algebra (loosely we can say that it is nothing else than an extension of the familiar spatial 3-D vector algebra to include any number of dimensions up to infinity); these mathematical aspects of the QM theory were summarized in the classic book by J. Von Neumann [3]. It is also worth noting that the QM's mathematical approach is also based on the analytical theory of classical mechanics as expressed by Hamilton-Jacobi theory*. Following the initial success in interpreting atomic spectroscopic data, the QM approach was applied to describe electromagnetic fields starting as early as 1927 as it is indicated by Dirac's pioneering work [4]. This project, a quantum theory of light, reached its peak with the development of quantum electrodynamics (QED) theory [5], added (and replacing) the only available theory of the time. This was the classical electromagnetic theory which had been growing the centuries past the 20th, compactly encompassed in the formulation of the four Maxwell's Equations.

Despite the huge success of QM it should be understood that the Copenhagen interpretation (or statistical interpretation) is still debatable as strong as it was 90 years ago; this because its assumptions, following logical steps, leads invevitably to a number of physical conclusions that have been proved difficult to gain general acceptance among the physics community. Among its eminent opponents are

1: [1] Bohr N, '*The Quantum Postulate and the Recent Development of Atomic Theory*', Nature, **121**, 580-590, (1928); W. Heisenberg '*The physical principles of the Quantum Theory*', (1930)
[2] Schrödinger, E. (1926). "*An Undulatory Theory of the Mechanics of Atoms and Molecules*", Phys. Review, **28**, 1049-1070, (1927)
[3] J. Von Neumann, '*Mathematical Foundations of Quantum Mechanics*', Princeton University Press, (1930)
[4] P. A. M. Dirac The Quantum Theory of the Emission and Absorption of Radiation, The Royal Society A, **114**, 243,(1927); P. A.M. Dirac, '*The principles of Quantum Mechanics*', Oxford Sciences Publication,
[5] S. Schweber, '*QED and the Men who made it: Dyson, Feynman, Schwinger, and Tomonaga*', (1994).
[6] Einstein A, Podolsky B, Rosen N., '*Can Quantum-Mechanical Description of Physical Reality Be Considered Complete?*', Phys. Rev. **47**, 777, (1935).
[7] E. Schrödinger, '*Die gegenwärtige Situation in der Quantenmechanik (The present situation in Quantum Mechanics)*' , Naturwissenschaften **23**, 807–812, (1935).

* Not normally taught in the early years of an undergraduate Physics program. This approach generalizes the Euler-Lagrange's equations of mechanics and is distinctly different from the Newton's approach based on the force/momentum concepts

Einstein and Schrödinger himself! Einstein never accepted QM's interpretation while in one of his most famous articles discussed the Einstein-Podolsky-Rosen paradox (*EPR paradox*) where some QM extreme conclusions were ingeniously surfaced [6]. On the other hand, at the same period Schrödinger expressed his own concerns which led to the so frequently quoted '*Schrödinger's cat paradox*' [7], so that any cat should be now aware of.

Nevertheless, despite the reservations on the QM theory, its principles have been the basis for the most accurate description of nature's (known) forces except *gravity*. To date, the two physical theories of the 20th century (Einstein's theory for gravity and QM) have not been able to be incorporated in a common physical framework as serious incompatibilities of their fundamental principles are in place.

QM is great because it is the most successful physical theory with regards to its applications to numerous fields of modern science in all physical scales in space (from the atomic world to the whole universe) and time accessible to experiment. It is worth to mention here that a recent (and rapidly) emerged field of applications in the area of quantum computation, communication and information science, frequently 'quantum technologies'. At the moment the quantum technologies research sector is heavily driven by major US/EU/China institutional bodies as well as from wealthy private vendors such as IBM,Google,Microsoft,Toshiba,Accenture etc.

In this module we'll study the QM principles using its 'natural' and most general mathematical formulation, namely, the Hilbert vector algebraic representation of the physical states and quantities. Within this viewpoint, the familiar $\psi(x)$ wavefunction is just a specialized mathematical representation of the state of quantum system (among other equivalent descriptions) with regard to its position in space. For clarification, this particular description contains no information about other physical properties of the quantum system (and therefore is of no use) with the most notable example the *spin* property (not to be confused with any actual spinning properties in the physical space).

Hilbert vector states 2

Traditionally, the first encounter with QM theory and its applications is not through the abstract Hilbert state vector formalism. Most likely, because the choice to present QM via the Schrödinger's wavefunction, $\psi(\mathbf{r})$ appears more familiar and has more direct links with classical mechanics (CM) theory and the every-day notion of a particle moving in the physical 3-D space; in CM the particle's position is given by the deterministic $\mathbf{r} = \mathbf{r}(t)$ while for QM a small step is required to replace this with the probability to find the particle in an elementary volume at each point, namely, to replace $\mathbf{r}(t) \to |\psi(\mathbf{r}, t)|^2 dV$. On the other hand the abstract state vector formalism is mathematically the most general and at a practical level, vastly, is the most economical one. The central concepts of this more general formulation for a physical system are (a) the physical states represented by a vector *state*, $|\psi\rangle$, (b) the observables represented by operators, $\hat{Q}$, and (c) the transformation rules when operators act on the vector states $\hat{Q}|\psi\rangle$, one deterministic and the other probabilistic; the former is a physical dynamics law for the state $|\psi\rangle$ (Schrödinger equation)) and the other describes the state's violent collapse when a *measurement* takes place. The mathematical properties of these quantities are those of a vector space (Hilbert) not very far different than the physical space vector space we are familiar with.

All the predictions about a QM system are derived from four central concepts, namely, the *abstract vector-states* $|\psi\rangle$ and the *observables-operator*s, $\hat{Q}$, the *Schrödinger equation* and the *measurement* dynamics laws.

There is no one definite set of QM postulates/principles/axioms; different authors, researchers, textbooks follow their own versions, according to their taste and possibly the context of presentation. Nevertheless, ultimately, all are in agreement each other as long as they follow the widely accepted to date, statistical (Copenhangen) interpretation of QM.

In the present text, my own preference of a minimal set of QM postulates, represents a merged version of the QM postulates as stated in their classic textbook by C. Cohen-Tannoudji, B. Diu an F. Laloë '*Quantum Mechanics*' :

2.1 Space vectors

The most general formulation of quantum mechanics (QM) is developed in terms of an abstract (Hilbert) vector space, which takes its name by the German mathematician David Hilbert (who have studied their properties extensively the past century). It will possibly help what if we revisit the vector space which is associated with the familiar 3-dimensional physical space. Following this review we'll go on and make suitable generalizations to arrive at a vector space where QM uses to express mathematically its statements about a quantum state and associated dynamical physical quantities (i.e. energy, momentum, spin, etc) of a physical system. In the below, unless otherwise state by physical system we mean quantum system and by physical state we mean quantum state (QS).

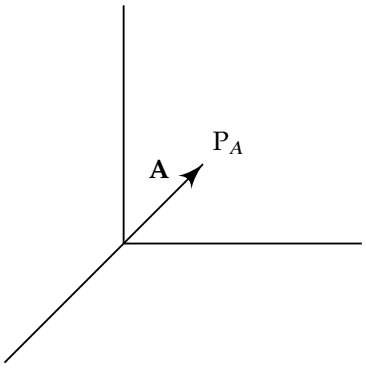

Figure 2.1: A vector in the physical space denoting point P_A.

3-D space vectors

[3] So let's represent the point of a space by a vector **A** which is characterized by two fundamental properties: *length* and *direction*.

We can re-scale a vector (increasing or decreasing its length) by a simple multiplication,

$$\mathbf{A}' = \lambda \mathbf{A}, \qquad \lambda \text{ real number}$$

This of course would mean that the tip of the vector would end to a different point, $P_{A'}$. Therefore the multiplication of **A** resulted to another vector $\mathbf{A}'$, also belonging in the physical vector space. This way, we can always determine the unit vector in the direction defined by the **A**, if we take $\lambda = 1/a$:

$$\hat{a} = \frac{\mathbf{A}}{a}, \qquad |\hat{a}| = 1. \tag{2.1}$$

Apart from its length, one may think an *operation* which alter its *direction*. How this can be generally done? At the moment we introduce a symbol which is used to represent this operation:

$$\hat{M}\mathbf{A} \to \mathbf{B} \qquad \hat{M} \textit{ operates (acts) on } \mathbf{A} \textit{ and transforms it to } \mathbf{B} \tag{2.2}$$

How in practice this *operation* takes place is left for later this after the introduction of a *reference* system (or *basis* system). For now, the reader should be prepared to think the vector **A** as a 3-element column and the *operator* $\hat{M}$ as a 3×3 matrix. The rescaling operation $a\mathbf{A}$, discussed earlier is just a special case of the above more general transformation process of **A**; namely it leaves the direction of **A** intact.

Addition operation. A single vector isn't very useful concept as it stands; so we should see what useful constructions and properties can be derived if the other similar vectors are added in the vector space. So we assume another vector **B**, pointing at P_B, which in general has different *length* and *direction*. Then we may *define* the *addition* operation

3:

Conventions

We use capital letters for vectors (bold) and operators (hat) belonging on the vector space (i.e. **A**, $\hat{M}$). Only exception are a vector of unit length which is denoted by a small letter with a hat. The length of the vector is denoted by the corresponding small letter. Therefore:

A	$\longleftrightarrow$ vector
a	$\longleftrightarrow$ length (= $\lvert\mathbf{A}\rvert$)
$\hat{a}$	$\longleftrightarrow$ unit vector along **A**
$\hat{M}$	$\longleftrightarrow$ Operator

which states that adding **A** and **B** and *new* vector is generated which of course it's characterized by its own l*ength* and *direction*. So if we name this vector as **C** we have [4] :

$$\mathbf{C} = \mathbf{A} + \mathbf{B}$$

The *addition* operation of two vectors is characterized by the following properties:

$$\begin{aligned} \mathbf{A} + \mathbf{B} &= \mathbf{B} + \mathbf{A}, \\ \mathbf{A} + (\mathbf{B} + \mathbf{C}) &= (\mathbf{A} + \mathbf{B}) + \mathbf{C} \\ \lambda(\mathbf{A} + \mathbf{B}) &= \lambda\mathbf{A} + a\mathbf{B}, \end{aligned}$$

Inner-product operation. One way to view this operation is as a measure of checking the 'parallelness' of any two vectors in other words how much their directions differ; For two vectors **A** and **B** this operation becomes maximum when they point in the same direction (*parallel*), minimum when they point to opposite directions (*anti-parallel*) and exactly zero when they are normal to each other (*orthogonal*). It takes any other value in between its extreme values for arbitrary relative directions. To quantify mathematically such information one can use the relative angle of the two vectors, Θ_{AB}:

Therefore, one way to define the inner product:

$$\mathbf{A} \cdot \mathbf{B} = AB \cos\Theta_{AB}, \qquad 0 \leq \theta \leq \pi, \tag{2.3}$$

Note that the *inner-product* is a *scalar* real-valued quantity.

Properties.

$$\begin{aligned} \mathbf{A} \cdot \mathbf{B} &= \mathbf{B} \cdot \mathbf{A} \\ \mathbf{A} \cdot (\mathbf{B} + \mathbf{C}) &= (\mathbf{A} \cdot \mathbf{B}) + \mathbf{A} \cdot \mathbf{C} \\ a(\mathbf{A} \cdot \mathbf{B}) &= (a\mathbf{A}) \cdot \mathbf{B} = \mathbf{A} \cdot (a\mathbf{B}) \end{aligned}$$

For parallel, anti-parallel and orthogonal **A**, **B** we have,

$$\mathbf{A} \cdot \mathbf{B} = \begin{cases} AB & \text{parallel} & \Theta_{AB} = 0 \\ -AB & \text{anti-parallel,} & \Theta_{AB} = 180^o \\ 0 & \text{orthogonal,} & \Theta_{AB} = 90^o \end{cases} \tag{2.4}$$

We may summarize at this point some basic facts for a vector space:

Objects in the vector space

So the physical vector space is constituted by *vectors*, (i.e. **A**) and *operators*, (i.e. $\hat{M}$). Vectors are characterized by their length and direction while the operators are defined by their action on the vectors.The operations of addition and inner-product are defined between two vectors, **A** and **B**. The former results to a new vector while the latter to a scalar value (it generally 'measures' the relative

4: It's also important to emphasize that: *the addition of two vectors results to a mathematical object with the same properties, namely, results to a vector*. For example in the physical space if **A** is used to characterize a point, P_a, the **B** to characterize a point, $\mathbf{P}_B$ then their addition $\mathbf{C} = \mathbf{A} + \mathbf{B}$ also characterizes a point P_C.

directionality of the two vectors). The action of the operator $\hat{M}$ on a vector **A** generally transforms the latter to a new one, **B**.

Cartesian coordinate system

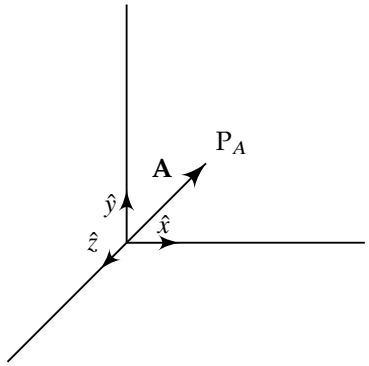

Figure 2.2: A Cartesian Coordinate System into physical space.

Now we have defined the vector algebra and some of the operations that can take place between different elements (i.e. between **A**, **B**, **C** etc) one can go further and work out various algebraic properties of the vector space. In many cases, instead of using symbolic mathematical operations it is convenient at some stage to introduce a method where these operations are represented by proper numerical algorithms, so that eventually can be numerically quantified. Such a method was introduced by Rene Descartes (it's called *analytical geometry method* where points in space are represented by numbers (i.e. a point in the 3-D space is represented by 3 numbers). So, recalling that our presentation here associates a vector with a point in a physical space it naturally results that, within this method, a vector is represented by 3 numbers, as well. For example, for points P_A,P_B, P_C we have,

$$\mathbf{A} \sim x_a, y_a, z_a \qquad \mathbf{B} \sim x_b, y_b, z_b \qquad \mathbf{C} \sim x_c, y_c, z_c, \quad \cdots$$

Complete and orthonormal basis $\hat{x}, \hat{y}, \hat{z}$. More specifically, a Cartesian Coordinate System (CCS) consists of three mutually orthogonal unit vectors, $\hat{x}, \hat{y}, \hat{z}$, of *fixed direction and origin*, independent on the particle's position:

$$\hat{x} \cdot \hat{y} = \hat{x} \cdot \hat{z} = \hat{y} \cdot \hat{z} = 0, \qquad \hat{x} \cdot \hat{x} = \hat{y} \cdot \hat{y} = \hat{z} \cdot \hat{z} = 1. \tag{2.5}$$

A practical (and compact) representation of these unit vectors is the column representation:

$$\hat{x} \equiv \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \qquad \hat{y} \equiv \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad \hat{z} \equiv \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix},$$

We can then define the rows to be $\hat{x}^T, \hat{y}^T, \hat{z}^T$:

$$\hat{x}^T \equiv \begin{pmatrix} 1, 0, 0 \end{pmatrix}, \qquad \hat{y}^T \equiv \begin{pmatrix} 0, 1, 0 \end{pmatrix}, \quad \hat{z}^T \equiv \begin{pmatrix} 0, 0, 1 \end{pmatrix}.$$

In this case the inner-products above can be calculated using matrix algebraic techniques. For example,

$$\hat{x} \cdot \hat{y} \equiv \hat{x}^T \cdot \hat{y} = \begin{pmatrix} 1, 0, 0 \end{pmatrix} \cdot \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = 0 + 0 + 0 = 0$$

and

$$\hat{x} \cdot \hat{x} \equiv \hat{x}^T \cdot \hat{x} = \begin{pmatrix} 1, 0, 0 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = 1 + 0 + 0 = 1$$

Orthonormal and complete vector basis

A basis like the one described above is orthonormal (since it is

defined by mutually *orthogonal unit* vectors. In addition we say that it is *complete* when every vector of the vector space can be written as a superposition of these three basis-vectors. We say that this basis *spans* the full vector space.

Vector components In view of the above property of the basis (here defines the Cartesian coordinate system $(Oxyz)$) $\mathbf{A}$ is fully determined by its three components along the axes (xyz), namely A_x, A_y, A_z in the following way:

$$\mathbf{A} = A_x\hat{x} + A_y\hat{y} + A_z\hat{z} \tag{2.6}$$

with length equal to,

$$a = \sqrt{A_x^2 + A_y^2 + A_z^2}, \tag{2.7}$$

So, the algebraic-representation $\mathbf{A}$ in the CCS Oxyz (or basis Oxyz) is a column-like vector:

$$\mathbf{A} = A_x\hat{x} + A_y\hat{y} + A_z\hat{z} \equiv A_x\begin{pmatrix}1\\0\\0\end{pmatrix} + A_y\begin{pmatrix}0\\1\\0\end{pmatrix} + A_z\begin{pmatrix}0\\0\\1\end{pmatrix} = \begin{pmatrix}A_x\\A_y\\A_z\end{pmatrix} \equiv A$$

Here we should make a clear-cut distinction between $\mathbf{A}$ and A contained in the above expressions:

$\mathbf{A}$ is the vector while A is its column representation in the specific reference system Oxyz (of the orthonormal basis $\hat{x}, \hat{y}, \hat{z}$).

These two describe the same object but are of different nature. $\mathbf{A}$ is invariant while A varies depending on the coordinate system, for if had we chosen a different CCS $Oxyz$ then we would have different numerical values for the same vector $\mathbf{A}$; For example, for a CCS $Ox'y'z'$ we would then have,

$$\mathbf{A} = \begin{pmatrix}A'_x\\A'_y\\A'_z\end{pmatrix} \equiv A',$$

with A' the column-representation of $\mathbf{A}$ in the primed reference system $Ox'y'z'$. Note though that since $\mathbf{A}$ is invariant its length remains the same and then *necessarily* we have,

$$a = \sqrt{(A'_x)^2 + (A'_y)^2 + (A'_z)^2} = \sqrt{A_x^2 + A_y r + A_z^2}$$

It should then be quite clear that when a matrix algebra is involved the numerical values are relative to a certain reference system (basis) and we should always be aware of it. [5]

Having clarifying the above, for the subsequent algebraic calculations it's convenient to define as A and its transpose of AT vector, as a 3-elements column and row representations of the same algebraic object,

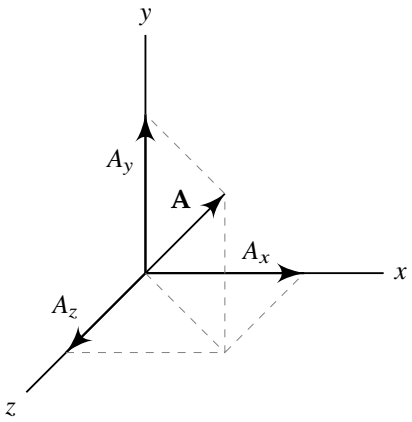

Figure 2.3: Cartesian components of a vector, (Oxyz).

5: The realization of this distinction is of vital importance for the understanding of the QM's abstract vector formalism, since each of the orthonormal basis is associated with a particular dynamical quantity of the quantum system (i.e. Spin along the 3 different spatial axes). Of course when only one basis is considered throughout the calculations there is no need to focus more on this distinction and very often the vector $\mathbf{A}$ is treated as identical to its associated column-representation A.

A :

$$A = \begin{pmatrix} A_x \\ A_y \\ A_z \end{pmatrix}, \qquad A^T = (A_x, A_y, A_z).$$

Note that both A and A^T qualify equivalently as entities to represent quantify **A** on the chosen reference system (basis).

Accordingly, we work if we want to perform any operation between two vectors **A** and **B**; we can analyze the operations to their corresponding components.

Addition operation For example if we want to add **A** and **B** the resulting vector **C** is given as:

$$\mathbf{C} = \mathbf{A} + \mathbf{B} = (A_x + B_x)\hat{x} + (A_y + B_y)\hat{y} + (A_z + B_z)\hat{z} = \begin{pmatrix} A_x \\ A_y \\ A_z \end{pmatrix} + \begin{pmatrix} B_x \\ B_y \\ B_z \end{pmatrix} = \begin{pmatrix} C_x \\ C_y \\ C_z \end{pmatrix}$$

Inner product (scalar) If the vectors **A and B** are expressed through their components A_x, A_y and B_x, B_y,

$$\mathbf{A} = A_x\hat{x} + A_y\hat{y} + A_z\hat{z}, \qquad \mathbf{B} = B_x\hat{x} + B_y\hat{y} + B_z\hat{z},$$

then inner product is given by:

$$\mathbf{A} \cdot \mathbf{B} = A_xB_x + A_yB_y + A_zB_z. \tag{2.8}$$

Finally from Eqns (2.3) and (2.8) we find that the angle θ between the vectors equal to [6] :

$$\cos\Theta_{AB} = \frac{\mathbf{A} \cdot \mathbf{B}}{AB} = \frac{A_xB_x + A_yB_y + A_zB_z}{AB}$$

In a matrix-representation of **A** in the basis of $\hat{x}, \hat{y}, \hat{z}$ we have,

$$\mathbf{A} \cdot \mathbf{B} \equiv A^T \cdot B = \begin{pmatrix} A_x, A_y, A_z \end{pmatrix} \cdot \begin{pmatrix} B_x \\ B_y \\ B_z \end{pmatrix} = A_xB_x + A_yB_y + A_zB_z$$

Matrix-vector product

In this section we are returning back to the problem of transformation of a vector **A** to another vector **B** as expressed symbolically by (2.2) $\hat{M}\mathbf{A} \rightarrow \mathbf{B}$. The task is how the operator **M** is materialized in a given reference system Oxyz (or equivalently the orthonormal basis, $\hat{x}, \hat{y}, \hat{z}$). It's not difficult to conclude that the operator takes the form of a 3×3 matrix:

$$M \cdot A = \begin{pmatrix} M_{11} & M_{12} & M_{13} \\ M_{21} & M_{22} & M_{23} \\ M_{31} & M_{32} & M_{33} \end{pmatrix} \cdot \begin{pmatrix} A_x \\ A_y \\ A_z \end{pmatrix} = \begin{pmatrix} M_{11}A_x + M_{12}A_y + M_{13}A_z \\ M_{21}A_x + M_{22}A_y + M_{23}A_z \\ M_{31}A_x + M_{32}A_y + M_{33}A_z \end{pmatrix} = \begin{pmatrix} B_x \\ B_y \\ B_z \end{pmatrix} = B$$

6: As a special case, the square amplitude of **A** can also be calculated:

$$\begin{aligned} \mathbf{A}^2 \equiv A^T \cdot A &= \begin{pmatrix} A_x, A_y, A_z \end{pmatrix} \cdot \begin{pmatrix} A_x \\ A_y \\ A_z \end{pmatrix} \\ &= A_xA_x + A_yA_y + A_zA_z \\ &= A_x^2 + A_y^2 + A_z^2. \end{aligned}$$

From the latter we obtain,

$$a = \sqrt{A_x^2 + A_y^2 + A_z^2}$$

Accordingly we can define the following operation for the transpose vectors of **A** and **B**:

$$\mathbf{A}^T \cdot \hat{M}' = \mathbf{B}^T$$

So the question to be answered here is: what is this mathematical object which represents the above vectorial operation? equivalently what is the matrix M' which if multiplied by the row $\mathbf{A}^T$ results to the row $\mathbf{B}^T$? It turns out that it is the *transpose* of M which gives [7] ,

$$A^T \cdot M^T = B^T .$$

7: The transpose of the matrix M^T is defined by swapping columns with rows:

$$M^T = \begin{pmatrix} M_{11} & M_{21} & M_{31} \\ M_{12} & M_{22} & M_{32} \\ M_{13} & M_{23} & M_{33} \end{pmatrix}$$

So, eventually, we have,

$$\left(A_x, A_y, A_z\right) \cdot \begin{pmatrix} M_{11} & M_{21} & M_{31} \\ M_{12} & M_{22} & M_{32} \\ M_{13} & M_{23} & M_{33} \end{pmatrix} = \left(B_x, B_y, B_z\right) \tag{2.9}$$

From the above considerations we can now highlight the below:

Matrix operators on an orthonormal basis

The operator, $\hat{M}$, acting on an arbitrary vector, **A** (represented as a column A) results to a new vector, **B** (represented by a column B) is represented as a square matrix with the same dimension as A and B (here 3×3. Accordingly the operator which acts on the $\mathbf{A}^T$ (represented as row A^T) and transforms it to the vector $\mathbf{B}^T$ (represented as a row B^T) is represented by the transpose matrix of M:

$$M \cdot A = B \quad \longleftrightarrow \quad A^T \cdot M^T = B^T$$

The eigenvalue problem: change of a basis (or a reference systems

One practical question which is often arise when dealing with algebraic calculations is how to define the reference system to express vectors, operators and associated operations (addition, inner-product, matrix-vector product, rotation of a vector, etc). Needless to say, that such choice can be radically affect the 'easiness' of the calculations but, for certain, the final result must be independent on the specific reference system choice. In the case of the physical space vector of 2-D or 3-D this task is certainly easier as we can easily envisage mutual orthogonal directions and choose the basis unit vectors along these directions. For higher dimensions this 'visual' construction does not apply. A more formal method, applicable to all cases is required here. Fortunately such a method is available and proceeds by considering the so-called matrix eigenvalue problem:

Eigenvalue problem

The matrix eigenvalue problem of a matrix M is as below:

$$M \cdot V = \lambda V, \qquad \text{Find the } \lambda \text{ and the } V. \tag{2.10}$$

The λ are called the *eigenvalues* of M and V are its *eigenvectors*.

Of course the above matrix eigenvalue problem has it's counterpart in the vector space using not their matrix/column representations but the vectors and the operator themselves:

$$\hat{M}\mathbf{V} = \lambda \mathbf{V} \tag{2.11}$$

From the above we see that given an operator $\hat{M}$ there is a special set of vectors (equicalently as special set of directions in space) where the *action* of the operator on these operators is only to re-scale them, with their direction unaffected. So for every operator each eigenvalue λ is associated with an eigenvector $\mathbf{V}$.

Going back to the matrix eigenvalue problem of (2.10) the important observation is the follow:

The eigenvectors of a symmetric matrix constitute an *orthogonal* and *complete* vector basis.

The latter properties mean that we can define an *orthonormal unit vector basis along the directions defined by the eigenvectors of any symmetric matrix on which any vector can be represented.* Or in other words (when we refer to the physical space) we can define a special Cartesian system of reference associated with any matrix.

Apart from the above considerations it remains the practical problem of how actually calculate eigenvalues and eigenstates of a given matrix, namely how we solve the matrix equation (2.10)? Maybe the best way to demonstrate the procedure is to present specific numerical examples. To this, the matrix eigenvalue problem for the matrix,

$$M = \begin{pmatrix} 3 & 2 & 0 \\ 2 & 2 & 2 \\ 0 & 2 & 1 \end{pmatrix}, \qquad M^T = M, \tag{2.12}$$

is relegated as an exercise. Additionally, an example of a 2×2 matrix diagonalization is presented in one of the questions.

Here we'll only present the outcomes of the solution which give for the eigenvalues and eigenstates of this matrix. Since it is a 3×3 matrix generally (unless the matrix is ill-posed) we expect 3 eigenvalues/eigen-

vectors:

$$M \cdot V_1 = \lambda_1 V_1, \qquad \leftrightarrow \qquad \lambda_1 = 5, \quad V_1 = \alpha_1 \begin{pmatrix} 2 \\ 2 \\ 1 \end{pmatrix},$$

$$M \cdot V_2 = \lambda_2 V_2, \qquad \leftrightarrow \qquad \lambda_2 = 2, \quad V_2 = \alpha_2 \begin{pmatrix} -2 \\ 1 \\ 2 \end{pmatrix},$$

$$M \cdot V_3 = \lambda_3 V_3, \qquad \leftrightarrow \qquad \lambda_3 = -1, \quad V_3 = \alpha_3 \begin{pmatrix} 1 \\ -2 \\ 2 \end{pmatrix},$$

with a_i, $, i = 1-2$ arbitrary numbers. Let's now take two of these eigenvectors and check whether (as claimed) orthogonal each other. For example,

$$V_1^T \cdot V_2 = \Big(2,2,1\Big) \cdot \begin{pmatrix} -2 \\ 1 \\ 2 \end{pmatrix} = \alpha_1\alpha_2 \left[(2)\times(-2) + 2\times 1 + 1\times 2\right] = \alpha_1\alpha_2(-4+4) = 0!$$

We'll let as an exercise for the reader to check whether indeed V_1, V_2, V_3 are *orthogonal* each other, that is:

$$V_i^T \cdot V_j = 0, \qquad i \neq j, \quad i,j = 1-3.$$

[8]

Having solved this eigenvalue problem we are now in a position where we can choose a reference system along the directions of the eigenvectors. One last step remains here to turn this basis from orthogonal to orthonormal. The eigenvectors generally are not normalized to unity, that is their length is not one (1) (i.e. $v_1 = \sqrt{|V_1|} = \alpha_1\sqrt{2^2+2^2+1^2} = 3\alpha_1$. But it's straightforward to normalize by a proper choice for each of the corresponding α_i. For example:

$$\hat{v}_1 = \frac{V_1}{v_1} = \frac{V_1}{3\alpha_1} = \frac{1}{3\alpha_1}\alpha_1 \begin{pmatrix} 2 \\ 2 \\ 1 \end{pmatrix} = \begin{pmatrix} 2/3 \\ 2/3 \\ 1/3 \end{pmatrix}.$$

Similar normalizations hold for the remaining two eigenvectors which eventually results to the following orthnormal eigenbasis:

$$\hat{v}_1 = \frac{1}{3}\begin{pmatrix} 2 \\ 2 \\ 1 \end{pmatrix} \qquad \hat{v}_2 = \frac{1}{3}\begin{pmatrix} -2 \\ 1 \\ 2 \end{pmatrix} \qquad \hat{v}_3 = \frac{1}{3}\begin{pmatrix} 1 \\ -2 \\ 2 \end{pmatrix}.$$

Their connection with the original fundamental basis of $\hat{x}, \hat{y}, \hat{z}$ is given

[8]:

A non-symmetric matrix

Consider the matrix

$$M = \begin{pmatrix} 33 & 16 & 72 \\ -24 & -10 & -57 \\ -8 & -4 & -17 \end{pmatrix} \tag{2.13}$$

Since it is a 3×3 matrix generally (unless the matrix is ill-posed) we expect 3 eigenvalues/eigenvectors. Convince yourself that these are given by:

$$\lambda_1 = 1, \quad V_1 = \begin{pmatrix} -15 \\ 12 \\ 4 \end{pmatrix},$$

$$\lambda_2 = 2, \quad V_2 = \begin{pmatrix} -16 \\ 13 \\ 4 \end{pmatrix},$$

$$\lambda_3 = 3, \quad V_3 = \begin{pmatrix} -4 \\ 3 \\ 1 \end{pmatrix}.$$

Of course, any multiply of the above eigenvectors qualify equally as solution of the corresponding eigenvalue problem. The point here is that these eigenvectors are not orthogonal each other, that is:

$$V_i^T \cdot V_j \neq 0, \quad i \neq j, i,j = 1-3.$$

by the corresponding vector elements, for example

$$\hat{v}_1 = \frac{2}{3}\hat{x} + \frac{2}{3}\hat{y} + \frac{1}{3}\hat{z}, \tag{2.14}$$

$$\hat{v}_2 = -\frac{2}{3}\hat{x} + \frac{1}{3}\hat{y} + \frac{2}{3}\hat{z}, \tag{2.15}$$

$$\hat{v}_3 = \frac{1}{3}\hat{x} - \frac{2}{3}\hat{y} + \frac{2}{3}\hat{z}. \tag{2.16}$$

This way we have constructed a new basis associated with a new reference system on which we can expand any vector or operator in the 3-D space! An interesting question to ask here is the following? How the original matrix M (represented on the basis of $\hat{x}, \hat{y}, \hat{z}$ (Oxyz reference system)) is represented on the basis of $\hat{v}_1, \hat{v}_2, \hat{v}_2$? The answer is that takes a diagonal structure with the diagonal elements being its eigenvalues:

Operator $\hat{M}$ represented on $\hat{x}, \hat{y}, \hat{z}$ as $\quad M$

Operator $\hat{M}$ represented on $\hat{v}_1, \hat{v}_2, \hat{v}_3$. $\quad M_D = \begin{pmatrix} 5 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & -1 \end{pmatrix}$,

Similar transformations hold for the representation of any arbitrary vector from the fundamental basis $\hat{x}, \hat{y}, \hat{z}$ to the new one (derived by the M matrix). In another words this is what we are rather familiar, thath the vector stays the same but its components change when a new basis considered (equivalently, a new reference system). For example one can calculate the representation of the vector ending to the point $P_A = (1, 1, 1)$ in the fundamental basis and in the basis of M. So,

$$A = \hat{x} + \hat{y} + \hat{z} = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \qquad \rightarrow \qquad A' = a_1\hat{v}_1 + a_2\hat{v}_2 + a_3\hat{v}_3 = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}$$

To solve this problem, one can make use of (2.14)-()2.15) to express $\hat{x}, \hat{y}, \hat{z}$ in terms of $\hat{v}_i$, $i = 1 - 3$ and substitute in the expression for A, above.

From the physical vector space to the QM vector space

All the above mathematical properties, defined in the physical vector space, are used by QM to formulate its principles. The QM's vector space is an extension of the physical vector space in the following way:

- The states are vectors with complex number components .
- The physical quantities are operators represented by complex (Hermitian) matrices

In addition to this extension a change of the vector notation is also applied in order to align with the so-called Dirac notation of the quantum states; nevertheless, still, mathematically are just members of the extended complex space of QM.

2.2 QM states (Vectors)

In analogy with the childhood vector algebra learned in high-school (or with the discourse of the previous section), the QM Hilbert's abstract vector space is of very similar nature with physical vector space; for example the Cartesian components of the familial position vector in a certain reference frame has its analogy in the Hilbert vector space in QM [see Fig. (2.4)].

More specifically, take **A** a vector in the physical 3D space. For smoother generalization of the concepts it's better to replace the notation of $\hat{x}, \hat{y}, \hat{z}$ to $\hat{x}_1, \hat{x}_2, \hat{x}_2$ instead. Then (Cartesian) components of **A** are (A_1, A_2, A_3) and the **A** itself is expressed along the three - orthogonal directions $(\hat{x}_1, \hat{x}_2, \hat{x}_3)$ as,

$$\mathbf{A} = \sum_{i=1}^{3} A_i \hat{x}_i, \qquad \hat{x}_i^T \cdot \hat{x}_j = \delta_{ij} \tag{2.17}$$

The last inner-product among the unit vectors $\hat{x}_i,\ i = 1-3$ is the *orthonormalization* condition required by any *orthonormalized* and *complete* basis. The meaning of *complete* means that all vectors of the space can be expanded on this basis.

Now, proceeding with the generalization of these concepts in QM let's make the following amendments in the notation. For the column-representation of $\hat{x}_i$ we change to:

$$\hat{x}_1 \quad \rightarrow \quad |x_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix},$$

$$\hat{x}_2 \quad \rightarrow \quad |x_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix},$$

$$\hat{x}_3 \quad \rightarrow \quad |x_3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix},$$

while for the row-representation of the transposed vectors, $\hat{x}_i^T$ we adopt the below notation:

$$\hat{x}_1^T \quad \rightarrow \quad \langle x_1| = \Big(1, 0, 0\Big),$$

$$\hat{x}_2^T \quad \rightarrow \quad \langle x_2| = \Big(0, 1, 0\Big),$$

$$\hat{x}_3^T \quad \rightarrow \quad \langle x_3| = \Big(0, 0, 1\Big).$$

Now the physical 3D vector $\mathbf{A} = (A_1, A_2, A_3)$ with A_i real, $(A_i = A_i^*), i = 1, 2, 3$ is re-expressed as,

$$A \quad \rightarrow \quad |A\rangle = A_1|x_1\rangle + A_2|x_2\rangle + A_3|x_3\rangle = \begin{pmatrix} A_1 \\ A_2 \\ A_3 \end{pmatrix}. \tag{2.18}$$

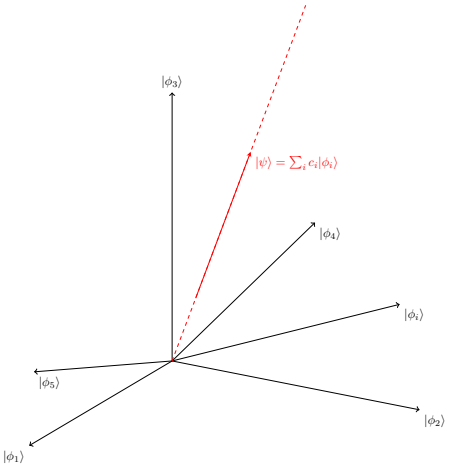

Figure 2.4: In quantum mechanics a physical state can be thought as a vector of the (abstract) Hilbert space spanned by the orthogonal eigenstates $|\phi_i\rangle$ of some observable operator, $\hat{Q}$. In accord to this geometrical picture any change of the state can be analyzed in terms of the observable's eigenstates which play the role of familiar components of linear algebra. In other words any observable defines its own 'coordinate system' for the vector state, known as *representation*.

So, the above expression isn't nothing more that (2.17) re-expressed with the new notation (which, in passing, is known in QM as *Dirac notation*). Now, if write down the row representation of **A** we should have something like,

$$A^T \qquad \rightarrow \qquad \langle A| = A_1^*\langle x_1| + A_2^*\langle x_2| + A_3^*\langle x_3| = \left(A_1^*, A_2^*, A_3^*\right).$$

Note that since the components are real, $A_i = A_i^*$ the use of A_i^* in A^T is still legitimate. In

Accordingly the inner-product of any two vectors **A** and **B** maybe now re-written as,

$$\mathbf{A}\cdot\mathbf{B} = A^T \cdot B = \langle A|\cdot|B\rangle \equiv \langle A|B\rangle$$

which in practice is evaluated using the decomposition of **A**, **B** as [9] ,

$$\langle A|B\rangle = A_1^*B_1 + A_2^*B_2 + A_3^*B_3 = \sum_{n=1-3} A_n^*B_n \tag{2.19}$$

9: again since we are still in the physical space the components A_i are real and thus $A_i = A_i^*$.

Till now, apart from the notational change to *Dirac* notation, nothing essential has been done and we are still in our familiar physical 3-D space (with all the good algebraic properties we know, i.e. vector addition, inner-product, vector decomposition etc).

Changes of essential nature will made now, so that the resulted space will have the properties that QM physical states obey, namely, the abstract Hilbert space.

– The vector components are extended to take complex values

$$A_i \qquad \rightarrow \qquad A_i = A_r + \imath A_i$$

This is the most fundamental change.

> *The vector space we have now is an abstract QM Hilbert space of dimension* 3.

– Allow the number of components to take any value between $n = 2, 3, \cdots N$, where N can be infinite.

> *The vector space we have then is an abstract QM Hilbert space of dimension* N.

With these generalizations we can write for an arbitrary vector $|\psi\rangle$ in this Hilbert space (*assuming* $A \rightarrow |\psi\rangle$ *and* $|x_i\rangle \rightarrow |v_i\rangle$), the generalizations of (2.18) and (2.19) as,

$$|\psi\rangle = \sum_n c_n|v_n\rangle = \begin{pmatrix} c_1 \\ c_2 \\ .. \\ c_n \\ .. \\ c_N \end{pmatrix}, \tag{2.20}$$

where, $|v_n\rangle$ are the corresponding unit vectors (which define the suitable orthogonal directions of this abstract space): [10] ,

$$|v_1\rangle = \begin{pmatrix}1\\0\\0\\..\\0\end{pmatrix}, \qquad |v_2\rangle = \begin{pmatrix}0\\1\\0\\..\\0\end{pmatrix}, \quad \cdots, \quad |v_n\rangle = \begin{pmatrix}0\\..\\1\\..\\0\end{pmatrix}, \quad |v_N\rangle = \begin{pmatrix}0\\0\\..\\0\\1\end{pmatrix},$$

$$\begin{aligned}
\langle v_1| &= \Big(1,0,0,..,0\Big),\\
\langle v_2| &= \Big(0,1,0,..,0\Big),\\
&\cdots\cdots\\
\langle v_n| &= \Big(0,..,1,..,0\Big),\\
\cdots&\cdots\\
\langle v_N| &= \Big(0,0,..,0,1\Big),
\end{aligned}$$

where we set $\mathbf{v}_i = |v_i\rangle$ and $\mathbf{v}_i^T = \langle v_i|$, $i = 1, 2, ...$ for the column and row vectors. For later reference let's call this (column) basis $(\{|v\rangle\} = |v_1\rangle, |v_2\rangle, ...)$ *fundamental ket basis* and its dual (row) basis as the *fundamental bra basis*. The above definitions help to express [11] : It's easily checked that the fundamental basis is orthonormalized,

$$\langle v_n|v_m\rangle = \delta_{nm} \tag{2.22}$$

Continuing with the generalization to the Hilbert space the conjugate vector of $|\psi\rangle$ (called *ket*) is denoted as $\langle\psi|$ (called *bra*) and is now represented by

$$\langle\psi| = \sum_n c_n^\star \langle v_n| = (c_1^*, c_2^*, \cdots, c_n^*, \cdots, c_N^*). \tag{2.23}$$

It is now immediately seen that the inner product of $|\psi\rangle$ with itself (multiplication of its bra with the ket state) which is nothing else but its *length* is evaluated as Alternatively, it can be calculated using the vector notation of (5.12) [12] ,

$$\langle\psi|\psi\rangle = \Big(c_1^*, ..., c_n^*, .., c_N^*\Big)\begin{pmatrix}c_1\\...\\c_n\\..\\c_N\end{pmatrix} = \sum_{n=1}^{N} |c_n|^2 \tag{2.24}$$

Certainly, the generalization of the familiar 3D algebra is slightly more involved for two reasons: (a) the dimensionality is higher (now it is not so easy to visualize a N mutually orthogonal vectors, $|v_n\rangle$, $n = 1, 2, \cdots, N$, and (b) generally the expansion coefficients and the inner-product are complex valued.

10: For example for a two-dimensional basis,

$$|v_1\rangle = \begin{pmatrix}1\\0\end{pmatrix}, \qquad |v_2\rangle = \begin{pmatrix}0\\1\end{pmatrix}.$$

and,

$$\langle v_1| = \Big(1,0\Big), \quad \langle v_2| = \Big(0,1\Big).$$

The orthonormalization property, $\langle v_i|v_j\rangle = \delta_{ij}$ is easily checked.

$$\langle v_1|v_1\rangle = \Big(1,0\Big)\cdot\begin{pmatrix}1\\0\end{pmatrix} = 1.$$

11: For a two-dimensional basis,

$$|\psi\rangle = \begin{pmatrix}c_1\\c_2\end{pmatrix}, \qquad \langle\psi| = \Big(c_1^*, c_2^*\Big). \tag{2.21}$$

12:

$$\begin{aligned}
\langle\psi|\psi\rangle = \langle\psi|\cdot|\psi\rangle &= \Big(\sum_n c_n^\star\langle v_n|\Big)\cdot\Big(\sum_m c_m|v_m\rangle\Big)\\
&= \sum_n\sum_m c_n^\star c_m \langle v_n|\cdot|v_m\rangle\\
&= \sum_n\sum_m c_n^\star c_m \langle v_n|v_m\rangle\\
&= \sum_n\sum_m c_n^\star c_m \delta_{nm} = \sum_n |c_n|^2.
\end{aligned}$$

The first QM principle Now we turn to first QM principle which states:

> The physical states of a quantum system are vectors of a multidimensional Hilbert vector state.

Then, let's assume from now on that when we say physical state $|\psi\rangle$ equivalent an abstract Hilbert vector state (following always the Dirac convention) represented either by its *ket* vector $|\psi\rangle$ or by its bra vector $\langle\psi|$ [13]. The $\mathcal{V}$ space is *linear* which affects radically its algebraic properties (and in turn of fundamental physical consequences); we say that a $\mathcal{V}$ is *linear* when *any linear combination of vector states belonging in* $\mathcal{V}$ *also belongs to* $\mathcal{V}$*, thus representing a physical state of the system*.

$$\text{if } |\chi\rangle,\ |\phi\rangle \text{ in } \mathcal{V} \quad \text{then} \quad |\psi\rangle = c_1|\chi\rangle + c_2|\phi\rangle \quad \text{in} \quad \mathcal{V}$$

Generally, a *complete* set of orthonormalized states $|\phi_n\rangle$ exists where all $|\psi\rangle$ in $\mathcal{V}$ can be expressed in a unique way as,

$$|\psi\rangle = \sum_n c_n|\phi_n\rangle, \qquad \langle\phi_n|\phi_m\rangle = \delta_{nm} \tag{2.25}$$

The above expansion is also known as *superposition expansion*. Also one should realize that the fundamental basis $|v_n\rangle$ it is not the only orthonormal basis to expand the $|\psi\rangle$ state [14]. *Any orthonormal basis will do equally*; the latter property is of vital importance in QM, especially in connection with its postulates related with the *dynamics* and the *measurement* of a physical state.

Moreover, since $\mathcal{V}$ is a complex-values linear vector space then (in analogy with the familiar physical vector space) an *inner-product* between any two vector states, $|\psi\rangle$ and $|\phi\rangle$, will be generally be complex number, and we denote it by [15],

$$\langle\psi|\phi\rangle \quad \text{understood as} \quad \langle\psi|\cdot|\phi\rangle$$

Its calculation in practice follows the standard inner-product rules as in (2.19), properly applied; therefore if $|\psi\rangle$ and $|\phi\rangle$ have as expansion coefficients $c_n, n = 1, 2, .., N$ and $d_m, m = 1, 2, ..., N$, respectively, then their inner-product is calculated numerically by,

$$\begin{aligned}\langle\psi|\phi\rangle &= \left(\sum_n c_m^\star\langle\phi_n|\right)\cdot\left(\sum_m d_m|\phi_m\rangle\right)\\ &= \sum_n\sum_m c_n^\star d_m\langle\phi_n|\phi_m\rangle = \sum_n c_n^\star d_n,\end{aligned}$$

where the orthonormalization condition of (2.25) $\langle\phi_n|\phi_m\rangle = \delta_{nm}$. [16] A special attention should be given to that QM is a probabilistic theory and its predictions should conform the probability laws restrictions; for this reason the states $|\psi\rangle$ should be properly normalized, that is,

13: Associated (isomorphically) with the vector space $\mathcal{V}$ there is the dual (abstract) vector space ($\mathcal{V}^\star$) containing all *bra* state ($\langle\psi|$) associated with each $|\psi\rangle$ of $\mathcal{V}$.

14: The same way where a physical vector can be expanded to different reference systems (corresponding to different bases). All these are discussed in the previous section.

15: **Exercises:** Let $|v_i\rangle$ be the fundamental basis.
1. Consider,

$$|\psi\rangle = |v_1\rangle + \imath|v_2\rangle, \qquad |\phi\rangle = |v_1\rangle - 3\imath|v_2\rangle$$

Calculate their inner products $\langle\phi|\psi\rangle$ and $\langle\psi|\phi\rangle$. Are these equal?
(hint: $\langle\psi|\phi\rangle = -2$).
2. Now take

$$|\psi\rangle = \imath|v_1\rangle + |v_2\rangle, \qquad |\phi\rangle = |v_1\rangle - 3\imath|v_2\rangle$$

Recalculate the corresponding inner products. Are they equal?
(hint: $\langle\psi|\phi\rangle = -4\imath$))

16: It also holds for the inner-product in the Hilbert space that,

$$\langle\psi|\phi\rangle = (\langle\phi|\psi\rangle)^*$$

should generally be unit Hilbert vectors, [17],

$$\langle\psi|\psi\rangle = \sum_{n=1}^{N} |c_n|^2 = 1. \tag{2.26}$$

Then we can summarize

A physical state of a system is represented by a normalized *vector* $|\psi\rangle$ belonging in some multidimensional linear complex vector space $\mathcal{V}$:

$$|\psi\rangle = \sum_n c_n|\phi_n\rangle, \qquad \langle\psi| = \sum_n c_n^\star\langle\phi_n|$$

where $|\phi_n\rangle$ is an orthonormalized basis for $\mathcal{V}$ generally complex. The latter property is known as *superposition principle*.

$$\langle\phi_n|\phi_m\rangle = \delta_{nm},$$

17: **Exercises**: Let $|v_i\rangle$ be the fundamental basis.
1. Consider,

$$|\psi\rangle = |v_1\rangle + \imath|v_2\rangle,$$

Is this a normalized state (Is its length equal to 1)?
2. Consider,

$$|\psi\rangle = \alpha|v_1\rangle + 2\imath|v_2\rangle,$$

Calculate α to normalize $|\psi\rangle$.
3. Now take

$$|\psi\rangle = \frac{\imath}{\sqrt{2}}(|v_1\rangle + |v_2\rangle), \quad |\phi\rangle = \frac{1}{\sqrt{10}}(|v_1\rangle - 3\imath|v_2\rangle)$$

Are the states above normalized. What are the values of their inner products? (hint: $\langle\psi|\phi\rangle = -2\imath/\sqrt{5}$))

2.3 QM observables and operators

Operators act on states. In QM operators are used to represent physical quantities, also known as *observables*. Examples are *energy*, *position*, linear and angular *momentum*, *spin*; more generally any combination of them is also an observable. The quantum expression of observables is obtained quite easily when the corresponding classical operator exists e.g. position ($\mathbf{r}$), linear and angular momentum ($\mathbf{p}$, $\mathbf{L}$), by following certain rules [18]. If one thinks that most of the classical mechanics quantities can be expressed in terms of position and momentum (e.g. angular momentum, $\mathbf{L} = \mathbf{r} \times \mathbf{p}$) then this approach covers a large number of cases. There are though cases where this route cannot be followed as for example the case of spin observable, which is a purely quantum quantity with no classical counterpart.

18: $\mathbf{x} \to \hat{x}$ and $\mathbf{p} \to -\imath\nabla$

In any case, each (quantum) observable is associated with an Hermitian operator in the corresponding Hilbert vector space. Also, Hermitian operators are represented in the vector space by Hermitian matrices. [19]. For example, an electron is associated with a spin observable where its z-component is represented by the 2×2 matrix:

$$S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

How the above matrix was constructed is not of our concern at the moment.

A very crucial property of Hermitian quantum operators is that they are associated with a set of orthogonal eigenvectors with *real* eigenvalues as:

Eigenbasis of an Hermitian operator (observable)

$$\hat{Q}|q_n\rangle = \lambda_n|q_n\rangle, \tag{2.27}$$

$$\langle q_n|q_m\rangle = \delta_{nm} = \begin{cases} 1 & n = m \\ 0 & n \neq m. \end{cases} \tag{2.28}$$

The eigenvalues λ_n are always real when the operator is Hermitian. Also this eigenbasis is *complete* which means that according to the superposition expansion (2.25) any ket state $|\psi\rangle$ can be expanded in terms of this eigenbasis as:

Expansion of a state on the observables eigenbasis

The eigenstates of any observable can be used as a basis to expand any state $|\psi\rangle$ of a quantum system according to the superposition principle:

$$|\psi\rangle = \sum_n c_n|q_n\rangle. \tag{2.29}$$

19: Hermitian operator is the operator which its matrix representation and its conjugate coincide. The conjugate of a matrix is obtained if we take its transpose and then we take its complex conjugate. Therefore,

$M^\dagger = (M^T)^*$ conjugate of M

Also for an Hermitian matrix:

$$M^\dagger = M.$$

Example, assume $M = \begin{pmatrix} 1 & 1 \\ -\imath & -1 \end{pmatrix}$ then,

$$M^\dagger = \begin{pmatrix} 1 & \imath \\ 1 & -1 \end{pmatrix}$$

The matrix operator $M = \begin{pmatrix} 2 & 1-2\mathbf{i} \\ 1+2\imath & 3 \end{pmatrix}$ is Hermitian because,

$$M^\dagger = \begin{pmatrix} 2^* & (1+2\mathbf{i})^* \\ (1-2\imath)^* & 3^* \end{pmatrix} = \begin{pmatrix} 2 & 1-2\mathbf{i} \\ 1+2\imath & 3 \end{pmatrix} = M$$

The coefficient c_n has a very precise algebraic meaning upon a measurement of $\hat{Q}$ [20]. For example assume we have the observable $\hat{Q}$ with eigenvalues λ_q and eigenstates $|q_n\rangle$. Also assume a second observable $\hat{Q}'$ with eigenvalues λ'_q and eigenstates $|q'_n\rangle$. Then the *same* state $|\psi\rangle$ can be expanded either as,

$$|\psi\rangle = \sum_n c_n |q_n\rangle,$$

or as

$$|\psi\rangle = \sum_n c'_n |q'_n\rangle,$$

These two different expansions correspond to the two different reference systems that can be used to expand the same physical vector, say **A**, in normal physical space. There the **A** takes two different component values A_x, A_y, A_z or A'_x, A'_y, A'_z depending on the reference system. Similar situation holds here. The two sets of expansion coefficients, c_n and c_n**'** (which are associated with each observable) are the 'components' of the same vector $|\psi\rangle$ in the two different bases.

20: Their physical meaning is defined with the QM postulate 3, later.

Action of an operator. The action of an observable in the state of a system needs to be determined here. The action of the operator on the *ket* vector of the states, $|\psi\rangle$, is determined by the use of (2.29) and (2.27) and (2.30). For example:

$$\hat{Q}|\psi\rangle = \hat{Q}\sum_n c_n |q_n\rangle = \sum_n c_n \hat{Q}|q_n\rangle = \sum_n c_n \lambda_n |q_n\rangle$$

Next remains the question about the action of the operator in the bra of the state, $\langle\psi|$:

$$\langle\psi|\hat{Q} = \sum_n c_n^\star \langle q_n|\hat{Q} = \sum_n c'_n \langle q_n|\hat{Q} = \sum_n c_n^\star \lambda_n \langle q_n|$$

For the last substitute we used the eigenvalue equation for the complex conjugate matrix of $\hat{Q}$

$$\begin{aligned} (\hat{Q}\cdot|q_n\rangle = \lambda_n|q_n\rangle)^\dagger \qquad &\rightarrow \qquad \langle q_n|\cdot(\hat{Q}^T)^* = \langle q_n|\lambda_n^* \\ \rightarrow \langle q_n|\hat{Q} = \lambda_n\langle q_n|, \qquad &\langle q_n|q_m\rangle = \delta_{nm}. \end{aligned} \tag{2.30}$$

where we set $\lambda_n = \lambda_n^*$ (since λ_n real)

A last note for here is that a further level of generalization arises when the basis is of infinite dimension. This is the case of observables which may take 'continuous' values such as position, momentum, energy in contrast to spin and angular momentum observables. Apart from the mathematical implications in general all the summations above turn to integrals.

2.4 Measurement

The action of an arbitrary operator, $\hat{Q}$, on a state $|\psi\rangle$ generally results to a different state, $\hat{Q}|\psi\rangle \rightarrow |\phi\rangle$. A measurement can be seen as a special type of time-evolution of a quantum system; the system changes abruptly state following its interaction with an external system (the measurement device). The measurement enforces a probabilistic time evolution of the system that is abrupt with a devastating effect in the system (known as '*collapse of the wavefunction*') ; Following measurement, regardless the state, only one state will survive. No deterministic predictions are possible within the generally accepted interpretation of a quantum measurement. It is exactly at this postulate that makes quantum mechanics an inherently probabilistic theory with no way to escape. A readable discussion about the various interpretations of quantum mechanics can be found in the book of S. Weinberg given in the prelude of these lectures (and references therein).

That said, let's now consider a system in a state $|\psi\rangle$ and an observable $\hat{Q}$. Assume the this state is written in terms of the eigenvectors of $\hat{Q}$, $|q_n\rangle$:

$$|\psi\rangle = \sum_n c_n |q_n\rangle.$$

A measurement of $\hat{Q}$ will give the real eigenvalue λ_n with probability, $P_\psi(\hat{Q} = \lambda_n) = |c_n|^2$ [21] . Since the measurements give results with some probability then it makes sense to define their average according to the standard definition:

$$\langle Q \rangle = \sum_n \lambda_n P_\psi(\lambda_n), \tag{2.31}$$

21: For short, $P_\psi(\lambda_n)$. This statement is known as *Born rule*. Let's interpret it as the probability a measurement of the observable OpQ to give the value λ_n when the system is in state $|\psi\rangle$.

An alternative more general expression is given by,

$$\langle Q \rangle = \langle \psi | \hat{Q}_n | \psi \rangle \tag{2.32}$$

The main difference between the two expressions for the average of the observable is that the use of (2.31) requires the knowledge of λ_n (so the eigenproblem should have been solved) while the use of (2.32) requires only the knowledge of $|\psi\rangle$ and $\hat{Q}$ on the same basis (here no any eigenvale problem is required). Obviously, depending on the problem one can use the most suitable expression.

Just after the measurement has taken place, then the system will have the state of the associated eigenvalue, namely, if the outcome was λ_n then the state of the system has taken the state $|\psi_n\rangle$. Subsequent measurements of $\hat{Q}$ will give again λ_n with certainty (probability 1). This not of surprise since we know that the system is in state $|\psi\rangle_n$. This irreversible measurement process where,

$$|\psi\rangle \qquad \text{Measurement of } \hat{Q} \qquad \rightarrow \qquad \text{gives } \lambda_n \text{ and system goes to state} \quad |q_n\rangle$$

is generally known as *collapse of the quantum state* (or reduction).

Measurement probabilities of observable $\hat{Q}$

The measurement of an observable $\hat{Q}$ when a physical system is in state $|\psi\rangle$ will result to one of the observables eigenvalues, λ_n with probability,

$$P_\psi(\mathbb{Q} = \lambda_n) = |c_n|^2 \tag{2.33}$$

The average value of the observable is given by

$$\langle Q\rangle_\psi = \langle\psi|\hat{Q}_n|\psi\rangle = \sum_n \lambda_n P_\psi(\lambda_n)$$

The state after the measurement is $|q_n\rangle$.

Subsequent measurement of $\hat{Q}$ will give again λ_n with certainty.

In the context of QM, the uncertainty in the measurement outcomes of $\hat{Q}$ when the system is in the state $|\psi\rangle$ is accordingly defined by [22]

$$(\Delta Q)_\psi \equiv \left[\langle\psi|(\hat{Q} - \langle\hat{Q}\rangle)^2|\psi\rangle\right]^{1/2}. \tag{2.34}$$

A more appropriate expression of is also given in terms of the averages of $\hat{Q}$ and $\hat{Q}^2$:

$$(\Delta\hat{Q})_\psi = \sqrt{\langle\hat{Q}^2\rangle - \langle\hat{Q}\rangle^2}, \tag{2.35}$$

where for simplicity, $\langle\hat{Q}^2\rangle_\psi \equiv \langle\psi|\hat{Q}^2|\psi\rangle$. According to these definitions the uncertainty in the measurements provides us a measure about the range of possible measurements around the average value, $\langle\hat{Q}\rangle_\psi$.

22: . The statistical measurements of a physical quantity will never give the same value. Due to imperfections of the measurements and fluctuations of the properties of the system under consideration, the outcomes will vary. Generally, the set of the outcomes is treated as a random variable, say X. We can always define an average result of the measurements. The spread of the results around its average value is quantified by the *standard deviation* (s.d)? The corresponding definitions from statistics is:

$$\bar{X} = \sum_{i=1}^{N} x_i \frac{\#\text{ of appearances}}{N}$$

$$\sigma_X = \left[\sum_{i=1}^{N}(x_i - \bar{X})^2\right]^{1/2}$$

where $\bar{X}$ is the average of the measurements.

2.5 Quantum dynamics (Schrödinger Equation)

The time-development of a quantum state assigns to the system's energy observable a special role, the most important among all the observables.

Assume a quantum system, with with the *energy* observable represented by the Hamiltonian $\hat{H}(t)$ operator. The QS is in the state described by the vector state $|\psi(t)\rangle$. QM postulates the following time-evolution law for the state $|\psi(t)\rangle$:

Dynamics of $|\psi\rangle$

$$\imath\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle, \qquad |\psi_0\rangle \equiv |\psi(t_0)\rangle. \tag{2.36}$$

The above fundamental law is known as time-dependent Schrödinger equation (TDSE). Since the TDSE includes the first derivative in time of the state, full specification of $|\psi(t)\rangle$ requires knowledge of the state at a fixed time t_0. [23]

23: You should always bear in mind that these equations for $|\psi(t)\rangle$ and $\hat{H}$ can always be thought as *matrix equations* between vectors and matrices.

It is important to appreciate that as long as the system, described by the $\hat{H}$, evolves in an isolated fashion (that is undisturbed), its time development is fully deterministic and its calculation is only of practical matter; exactly of the same nature as the one encountered in the classical theories mechanics and electrodynamics. The deterministic QM time-evolution law is interrupted when a measurement takes place (that is the system is disturbed). The measurement process is an inherently probabilistic time-evolution law, in sharp contrast with the TDSE law's very nature.

2.6 QM Principles summarized

Needless to say, a lot more remains to be said about QM but surely the below summary may be used as a minimal reference set of principles apllied in one form or another. [24]

A minimal set of QM postulates

1 **States.** *A physical state* of a system is represented by a normalized *vector* $|\psi\rangle$ belonging in some multidimensional linear complex vector space $\mathcal{V}$:

$$|\psi\rangle = \sum_n c_n |\phi_n\rangle, \qquad \langle\phi_n|\phi_n\rangle = \delta_{nm} \tag{QM1}$$

where $|phi_n\rangle$ is a basis for $\mathcal{V}$ and c_n generally complex. The latter property is known as *superposition principle*.

2 **Observables.** *A physical quantity* is represented by an *observable* $\hat{Q}$, which defines a *complete, orthonormalized*, eigenbasis $|q_n\rangle$ of $\mathcal{V}$ via its *eigenvalue equation* [25] :

$$\hat{Q}|\lambda_n\rangle = q_n|q_n\rangle \quad \rightarrow \quad \begin{cases} q_n & \text{real,} \\ \langle q_n|q_m\rangle & = \delta_{nm} \end{cases} \tag{QM2}$$

The latter two equations are known as *completeness* and *orthonormalization* conditions, respectively.

3 **Measurement of an observable.** A measurement [26] of an observable $\hat{Q}$ in state $|\psi\rangle$ gives one of its eigenvalues q_n with probability:

$$|\psi\rangle = \sum_n c_n |q_n\rangle \quad \rightarrow \quad P_\psi(\mathbb{Q} = q_n) = |c_n|^2 \tag{QM3}$$

The average and the uncertainty (standard deviations) of the measurements outcomes are:

$$\langle Q\rangle_\psi = \langle\psi|\hat{Q}_n|\psi\rangle, \qquad (\Delta\hat{Q})_\psi = \sqrt{\langle\hat{Q}^2\rangle - \langle\hat{Q}\rangle^2}$$

The post-measurement state of the system is $|q_n\rangle$ with certainty. This QM process is also known as *reduction (or collapse)* of the state.

4 **Dynamics of a state.** The time evolution of the state $|\psi\rangle$ is governed by the system's Hamiltonian, $\hat{H}$,

$$\imath\hbar\frac{d}{dt}|\psi\rangle = \hat{H}|\psi\rangle. \tag{QM4}$$

The latter form is known as Schrödinger Equation .

24: Note that classical and electrodynamics theories are also based on a small number of governing laws. For example, for mechanics that is the 3 Newton's laws (or, most correctly the fundamental, Euler-Langrange/Hamilton principle) and for electrodynamics the 4 Maxwell's laws.

25: An adjustment of the formulation should be made in the case where the observable are of continuous nature (e.g. position,momentum, etc), namely, when the eigenvalues q_n are no longer discrete.

26: This postulate concerns an *ideal* measurement where the effects of the measurements process (via the interaction with the (classical) apparatus) are minimal. The measurement process is of particular importance as it departs from a purely QM deterministic description of nature (Shrödinger Equation) toward an inherently probabilistic description due to interaction with the (external) measurement device. The main problem lies that the measuring process involves a classical system (measuring device) which is not described by the QM theory. This postulate has been the subject of continuous debate since the QM's inception. The present *statistical* interpretation (also known as the *Copenhagen* interpretation) was put forward by N. Bohr, W. Heisenberg, Max Born and their colleagues during the years of 1925-27.

2.7 Examples

Question 2.7.1

Assume, a system in the state $|\psi\rangle = N(|1\rangle + |2\rangle + |3\rangle)$ with $|i\rangle, i = 1-3$ orthonormalized, complete basis. [27] Calculate an acceptable value for the N.

27: Since the dimension is $N = 3$ the fundamental basis vectors $|i\rangle$ represented algebraically as:

$$|1\rangle = \begin{pmatrix}1\\0\\0\end{pmatrix}, \quad |2\rangle = \begin{pmatrix}0\\1\\0\end{pmatrix}, \quad |3\rangle = \begin{pmatrix}0\\0\\1\end{pmatrix}.$$

In addition for $N = 2$ the fundamental basis is defined by:

$$|1\rangle = \begin{pmatrix}1\\0\end{pmatrix}, \quad |2\rangle = \begin{pmatrix}0\\1\end{pmatrix},$$

In both cases, the definitions fulfills the orthonormalization requirements:

$$\langle i|j\rangle = \delta_{ij}$$

Solution: In the below, two different mathematical manipulation approaches are used to arrive at the answer. Let's call the first one, the *algebraic* method and the other the *operational* method. In the *algebraic* method we express the quantum states and observables in a row,column or matrix form and perform the calculations while in the *operational* approach we use symbolic representation of the states (i.e. $|\psi\rangle$ and observables $\hat{Q}$.

Algebraic method (matrix algebra) In accord to (QM1) the state $|\psi\rangle$ must be normalized:

$$\langle\psi|\psi\rangle = 1$$

Then, since,

$$|\psi\rangle = N|1\rangle + N|2\rangle + N|3\rangle = \begin{pmatrix}N\\N\\N\end{pmatrix}$$

we calculate the magnitude of the state, $|\psi\rangle$ by taking the inner product with itself as [28]

$$\langle\psi|\psi\rangle = \underbrace{\left(N^*, N^*, N^*\right)}_{\langle\psi|} \cdot \underbrace{\begin{pmatrix}N\\N\\N\end{pmatrix}}_{|\psi\rangle} = N^*N + N^*N + N^*N = 3|N|^2 = 1$$

28: We do this the same way as in the normal physical space of vectors, i.e. if we have a space vectors $\mathbf{A} = a_x\hat{x} + a_y\hat{y} + a_z\hat{z}$ then its magnitude is,

$$\begin{aligned}\mathbf{A}^2 &= \mathbf{A}\cdot\mathbf{A} = (a_x, a_y, a_z)\cdot(a_x, a_y, a_z)\\ &= a_x^2 + a_y^2 + a_z^2\\ &\rightarrow A = \sqrt{a_x^2 + a_y^2 + a_z^2}\end{aligned}$$

Then, from the above we have,

$$3|N|^2 = 1 \qquad \rightarrow \qquad N = \frac{e^{\imath\phi}}{\sqrt{3}}.$$

We cannot specify further the N. We are able to know only its *length* which, in any case, according to QM is the only property that matters. In other a *single* quantum state can be defined up to an arbitrary phase factor. For example we can simplify and choose $\phi = 0$ and therefore,

$$\boxed{N = \frac{1}{\sqrt{3}}}.$$

But it's important to understand that the choice $N = \imath/\sqrt{3}$ or $N = -\imath/\sqrt{3}$ are equally valid; or any other choice provided that the length of $|\psi\rangle$ is the unity.

Operational method Again in accord to (QM1) we may the superposition expansion of the state $|\psi\rangle$ on the eigenbasis (in its ket form)

is,

$$|\psi\rangle = \sum_{n=1-3} c_n|i\rangle = c_1|1\rangle + c_2|2\rangle + c_3|3\rangle,$$

or in its bra form:

$$\langle\psi| = \sum_{n=1-3} c_n^*\langle i| = c_1^*\langle 1| + c_2^*\langle 2| + c_3^*\langle 3|,$$

Then the $\langle\psi|\psi\rangle$ is nothing else than the inner product between the 'vectors' $\langle\psi|$ and $|\psi\rangle$. In the particular case we have $c_1 = c_2 = c_3 = N$ and the above requirement gives,

$$\begin{aligned}
\langle\psi|\psi\rangle &= \underbrace{(c_1^*\langle 1| + c_2^*\langle 2| + c_3^*\langle 3|)}_{\langle\psi|} \cdot \underbrace{(c_1|1\rangle + c_2|2\rangle + c_3|3\rangle)}_{|\psi\rangle} = \\
&= c_1^*c_1\cancelto{1}{\langle 1|1\rangle} + c_2^*c_2\cancelto{1}{\langle 2|3\rangle} + c_3^*c_3\cancelto{1}{\langle 3|3\rangle} \\
&+ c_1^*c_2\cancelto{0}{\langle 1|2\rangle} + c_1^*c_3\cancelto{0}{\langle 1|3\rangle} + c_2^*c_1\cancelto{0}{\langle 2|1\rangle} \\
&+ c_2^*c_3\cancelto{0}{\langle 2|3\rangle} + c_3^*c_1\cancelto{0}{\langle 3|1\rangle} + c_3^*c_2\cancelto{0}{\langle 3|2\rangle} \\
&= N^*N + N^*N + N^*N = 3|N|^2 = 1.
\end{aligned}$$

From this point we can continue as worked in the algebraic method to find $N = 1/\sqrt{3}$. Note in order to arrive in the final expression,the orthnormalization properties of the eigenbasis was used,

$$\langle i|j\rangle = \delta_{ij} = \begin{cases} 1, & i = j, \\ 0, & i \neq j. \end{cases}$$

NOTE: Of course you do not need to do all the job above to evaluate the inner product of two QM vectors $\langle\psi_A|\psi_B\rangle$. If the two vectors are expanded on a eigenbasis $\{|i\rangle\}$ $i = 1, 2, \cdots N$ (which means orthonormalized) i.e. $\psi_A = \sum_i a_i|i\rangle$ and $\psi_B = \sum_i b_i|i\rangle$ then we can immediately write:

$$\langle\psi_A|\psi_B\rangle = \sum_i a_i^*b_i$$

In our case, we could have written immediately,

$$\langle\psi|\psi\rangle = |c_1|^2 + |c_2|^2 + |c_3|^2 = 3|N|^2.$$

Question 2.7.2

A system is prepared in the state

$$|\psi\rangle = \frac{e^{\imath\phi}}{\sqrt{3}}|s_1\rangle + \imath\sqrt{\frac{2}{3}}|s_2\rangle,$$

where the $|s_1\rangle, |s_2\rangle$ are the eigenstates of the $\hat{S}_z$ observable, taken as, The ket basis is represented by the spin-fundamental vectors

$(|s_1\rangle, |s_2\rangle)$:

$$|s_1\rangle = |2\rangle = \begin{pmatrix}0\\1\end{pmatrix}, \qquad |s_2\rangle = |1\rangle = \begin{pmatrix}1\\0\end{pmatrix}.$$

Upon a measurement of the $\hat{S}_z$ observable
(a) what are the possible outcomes and
(b) calculate the probability for each outcome.
(c) What is the average (mean value or expectation value) for the observable?
(d) Assuming that the measurement shows the value $S_z = +\hbar/2$ what is the state of the system immediately after the measurement?

Solution.

(a) According to QM, the eigenstates of any spin observable can be used to expand any arbitrary state of a spin state of the system:

$$|\psi\rangle = c_1|s_1\rangle + c_2|s_2\rangle, \qquad |\psi\rangle \textit{ represents a spin state}$$

In our case here, the spin observable is the $\hat{S}_y$ and therefore $|s_1\rangle, |s_2\rangle$ are its eignestates:

$$\hat{S}_z|s_1\rangle = -\frac{\hbar}{2}|s_1\rangle, \qquad \hat{S}_z|s_2\rangle = \frac{\hbar}{2}|s_2\rangle. \qquad \textit{Eigenvalue equations for } \hat{S}_z$$

In the above, the state $|s_1\rangle$ is associated with the negative eigenvalue, $\lambda_1 = -\hbar/2$ of the $\hat{S}_z$ and $|s_2\rangle$ with the positive eigenvalue $\lambda_2 = \hbar/2$.
According to (QM3) postulate the possible measurement outcomes of the observable $\hat{S}_z$ are its eigenvalues. So, we expect only the values $\pm\hbar/2$ as the only outcomes.

(b) Comparing the expression of the state $|\psi\rangle$ on an eigenstate basis, (2.29), with the given expression (on the two-dimensional $\hat{S}_z$ eigenstate basis) we obtain the expansion c_1, c_2 coefficients:

$$|\psi\rangle = c_1|s_1\rangle + c_2|s_2\rangle \qquad \Longrightarrow \qquad \begin{cases} c_1 = \frac{e^{\imath\phi}}{\sqrt{3}} \\ c_2 = \imath\sqrt{\frac{2}{3}} \end{cases}$$

Since the state $|\psi\rangle$ is expanded on the S_z eigenbasis. In accord to QM postulate, (QM3), a measurement of $\hat{S}_z$ will provide the eigenvalue of $\lambda_1 = -\hbar/2$ with probability:

$$P_1(S_z = -\frac{\hbar}{2}) = |c_1|^2 = \left|\frac{e^{\imath\phi}}{\sqrt{3}}\right|^2 = \frac{1}{3}. \tag{2.37}$$

In the above it was used, $|e^{\imath\phi}|^2 = 1$). The positive eigenvalue, $\lambda = +\hbar/2$ will be found with probability:

$$P_2(S_z = \frac{\hbar}{2}) = |c_2|^2 = \left|\imath\sqrt{\frac{2}{3}}\right|^2 = \frac{2}{3} \tag{2.38}$$

since $|\imath|^2 = 1$.

(c) The mean average value of $\hat{S}_z$ is (by definition of the average)

$$\langle S_z\rangle = \lambda_1 P_1 + \lambda_2 P_2 = \lambda_1|c_1|^2 + \lambda_2|c_2|^2 = (-\frac{\hbar}{2})\frac{1}{3} + (\frac{\hbar}{2})\frac{2}{3} = \frac{\hbar}{6}$$

Question 2.7.3

The spin-x observable of the electron spin is represented as the 2×2 matrix,

$$\hat{S}_x = \frac{\hbar}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}. \tag{2.39}$$

This representation is based on the eigenbasis of the $\hat{S}_z$ observable. Calculate the value of $\langle s_1|\hat{S}_x|s_2\rangle$, where $|s_i\rangle$ is the spin-fundamental basis defined earlier.

Solution: Since the $\hat{S}_x$ observable is represented by a 2×2 matrix so the dimension of the vector space is $n = 2$. We can most easily evaluate $\langle 1|\hat{S}_x|2\rangle$ by using the *algebraic* method. Then, $\langle s_1|$ is a row-2 vector, $\hat{S}_x$ a 2×2 matrix $|s_2\rangle$ a column-2 vector:

$$\begin{aligned}\langle s_1|\hat{S}_x|s_2\rangle = \langle s_1|\cdot\hat{S}_x\cdot|s_2\rangle &= \underbrace{\begin{pmatrix}0,1\end{pmatrix}}_{\langle s_1|}\cdot\underbrace{\frac{\hbar}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}}_{\hat{S}_x}\cdot\underbrace{\begin{pmatrix}1\\ 0\end{pmatrix}}_{|s_2\rangle}\\ &= \begin{pmatrix}0,1\end{pmatrix}\cdot\frac{\hbar}{2}\begin{pmatrix}0\times 1+1\times 0\\ 1\times 1+0\times 0\end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix}0,1\end{pmatrix}\cdot\begin{pmatrix}0\\ 1\end{pmatrix}\\ &= \frac{\hbar}{2}(0\times 0+1\times 1) = \frac{\hbar}{2}\end{aligned}$$

From the latter expression comparison with (2.39) gives [29]

$$\boxed{\langle s_1|\hat{S}_x|s_2\rangle = \frac{\hbar}{2}.}$$

29: Convince yourself that if instead you had asked to evaluate, $\langle 2|\hat{S}_x|1\rangle$ on the fundamental basis $|1\rangle, |2\rangle$ you would have obtained the same value:

$$\langle 2|\hat{S}_x|1\rangle = \frac{\hbar}{2}$$

Note that $|s_1\rangle = |2\rangle$ and $|s_2\rangle = |1\rangle$.

Question 2.7.4

Consider the subquestion (d) of Question (2.7.2) and calculate the quantum average of $\hat{S}_z$ by use of the following expression:

$$\langle\hat{S}_z\rangle = \langle\psi|\hat{S}_z|\psi\rangle$$

Solution: The *ket* representation of the state ψ in the $\hat{S}_z$ basis of $|s_1\rangle, |s_2\rangle$ are as below:

$$|\psi\rangle = \frac{e^{\imath\phi}}{\sqrt{3}}|s_1\rangle + \imath\sqrt{\frac{2}{3}}|s_2\rangle = \frac{e^{\imath\phi}}{\sqrt{3}}\begin{pmatrix}0\\ 1\end{pmatrix} + \imath\sqrt{\frac{2}{3}}\begin{pmatrix}1\\ 0\end{pmatrix} = \begin{pmatrix}\imath\sqrt{\frac{2}{3}}\\ \frac{e^{\imath\phi}}{\sqrt{3}}\end{pmatrix}.$$

Accordingly, the *bra* representation of the state ψ is

$$\langle\psi| = \frac{e^{-\imath\phi}}{\sqrt{3}}\langle 1| + (-\imath\sqrt{\frac{2}{3}})\langle 2|) = \frac{e^{-\imath\phi}}{\sqrt{3}}\begin{pmatrix}01\end{pmatrix} - \imath\sqrt{\frac{2}{3}}\begin{pmatrix}10\end{pmatrix} = \begin{pmatrix}-\imath\sqrt{\frac{2}{3}}, \frac{e^{-\imath\phi}}{\sqrt{3}}\end{pmatrix}.$$

Now we are ready to use the given formula for the average:

$$\begin{aligned}\langle S_z\rangle = \langle\psi|\hat{S}_z|\psi\rangle = \langle\psi|\cdot\hat{S}_z\cdot|\psi\rangle &= \underbrace{\begin{pmatrix}-\imath\sqrt{\frac{2}{3}}, \frac{e^{-\imath\phi}}{\sqrt{3}}\end{pmatrix}}_{\langle\psi|}\cdot\underbrace{\frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}}_{\hat{S}_z}\cdot\underbrace{\begin{pmatrix}\imath\sqrt{\frac{2}{3}}\\ \frac{e^{\imath\phi}}{\sqrt{3}}\end{pmatrix}}_{|\psi\rangle}\\ &= \frac{\hbar}{2}\begin{pmatrix}-\imath\sqrt{\frac{2}{3}}, \frac{e^{-\imath\phi}}{\sqrt{3}}\end{pmatrix}\cdot\begin{pmatrix}\imath\sqrt{\frac{2}{3}}\\ -\frac{e^{\imath\phi}}{\sqrt{3}}\end{pmatrix} = \frac{\hbar}{2}\left[(-\imath\sqrt{\frac{2}{3}})\times(\imath\sqrt{\frac{2}{3}}) + \frac{e^{-\imath\phi}}{\sqrt{3}}\times(-\frac{e^{\imath\phi}}{\sqrt{3}})\right]\\ &= \frac{\hbar}{2}\left[-\imath^2\frac{2}{3} + |e^{\imath\phi}|^2(-\frac{1}{3})\right] = \frac{\hbar}{2}(\frac{2}{3} - \frac{1}{3}) = \frac{\hbar}{6},\end{aligned}$$

since $\imath^2 = -1$ and $|e^{\imath\phi}|^2 = 1$. This values coincides with the one calculated in Eq. (28).

Question 2.7.5

In QM the Energy observable is represented by the Hamiltonian operator, $\hat{H}$. For a quantum system its representation on an eigenbasis $|v_1\rangle, |v_2\rangle$

$$\hat{H} = E_0\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}, \qquad E_0 > 0,$$

The state of the system is $|\psi\rangle = |v_1\rangle$.

Upon measurement of the energy of this system find:

(a) The possible energy values

(b) the probability that the energy measurement will give the lowest possible value.

Solution. To solve this question we should proceed by

- finding the eigenspectrum of the Hamiltonian (eigenstates/eigenvalues) say $|\phi_1\rangle, |\phi_2\rangle$,

- use QM postulate (QM3) and expand the *fundamental* state $|1\rangle$ on the Hamiltonian's eigenbasis to find the probability for an energy measurement resulting to a negative value.

(a) *(Eigenstates/eigenvalues) of $\hat{H}$.*
The eigenvalue equation for the Hamiltonian is,

$$\hat{H}|\phi\rangle = \epsilon|\phi\rangle, \tag{2.40}$$

Denoting the fundamental basis vectors as,

$$|v_1\rangle = |1\rangle = \begin{pmatrix}1\\0\end{pmatrix}, \qquad |v_2\rangle = |2\rangle = \begin{pmatrix}0\\1\end{pmatrix}. \tag{2.41}$$

the $|\phi\rangle$ is represent by a the column vector,

$$|\phi\rangle = c_1|1\rangle + c_2|2\rangle = \begin{pmatrix}c_1\\c_2\end{pmatrix}. \tag{2.42}$$

Then by replacing with the given matrix-representation of the Hamiltonian's, the eigenvalue equation, (2.40), is turned to an 2×2 algebraic (matrix-diagonalization) problem.

$$\begin{aligned} E_0\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}\begin{pmatrix}c_1\\c_2\end{pmatrix} = \epsilon\begin{pmatrix}c_1\\c_2\end{pmatrix} \quad &\rightarrow \quad \begin{pmatrix}E_0 & E_0\\ E_0 & -E_0\end{pmatrix}\begin{pmatrix}c_1\\c_2\end{pmatrix} = \epsilon\begin{pmatrix}c_1\\c_2\end{pmatrix} \\ \rightarrow \quad \begin{pmatrix}E_0-\epsilon & E_0\\ E_0 & -E_0-\epsilon\end{pmatrix}&\begin{pmatrix}c_1\\c_2\end{pmatrix} = 0. \end{aligned} \tag{2.43}$$

The above 2×2 problem has a solution only if the matrix's determinant, $D(\epsilon) = det(M(\epsilon))$ is zero. [30] This requirement will give the possible eigenvalues:

$$\begin{aligned} &D(\epsilon) = 0 \qquad \rightarrow \\ &D(\epsilon) = -(E_0-\epsilon)(E_0+\epsilon) - E_0^2 = -(E_0^2-\epsilon^2) - E_0^2 \\ &\qquad = 2E_0^2 - \epsilon_2 = 0 \\ \rightarrow \quad &\boxed{\epsilon_1 = -E_0\sqrt{2}, \qquad \epsilon_2 = E_0\sqrt{2}} \end{aligned}$$

Calculation of eigenstate with $\epsilon_2 = E_0\sqrt{2}$. In this case by replacing ϵ_2 in (2.43) we have,

$$\begin{aligned} \begin{pmatrix}E_0 - E_0\sqrt{2} & E_0\\ E_0 & -E_0 - E_0\sqrt{2}\end{pmatrix}\begin{pmatrix}c_1\\c_2\end{pmatrix} = 0, \quad &\rightarrow \\ E_0\begin{pmatrix}1-\sqrt{2} & 1\\ 1 & -1-\sqrt{2}\end{pmatrix}\begin{pmatrix}c_1\\c_2\end{pmatrix} = 0 \quad &\rightarrow \\ c_1(1-\sqrt{2}) + c_2 = 0 \quad &\text{(2.44a)} \\ c_1 - c_2(1+\sqrt{2}) = 0 \quad &\text{(2.44b)} \end{aligned}$$

Equations (2.44a)-(2.44b) are equivalent (so only one can be used) [31] and therefore in order to find c_1 and c_2 we need one more equations. This equation is of physical nature in the sense that it is provided by the QM requirement that the state of a system should be normalized to unity:

$$\langle\phi|\phi\rangle = \left(c_1^*, c_2^*\right)\cdot\begin{pmatrix}c_1\\c_2\end{pmatrix} = |c_1|^2 + |c_2|^2 = 1, \tag{2.45}$$

So picking the latter equation and *any* of the equations (2.44a)-(2.44b) we can solve for c_1, c_2. For example picking (2.44a) we

30: $$M(\epsilon) = \begin{pmatrix}E_0-\epsilon & E_0\\ E_0 & -E_0-\epsilon\end{pmatrix}$$

31: Multiply (2.44b) by $1-\sqrt{2}$ and you'll see that (2.44a) is obtained.

have,

$$c_1(1-\sqrt{2})+c_2=0, \qquad |c_1|^2+|c_2|^2=1,$$

one easily can arrive at,

$$|c_1|=\frac{1}{\sqrt{2(2-\sqrt{2})}} \qquad \rightarrow \qquad c_1=\frac{e^{\imath\theta}}{\sqrt{2(2-\sqrt{2})}} \qquad \theta \text{ arbitrary.}$$

For simplicitly we choose $\theta=0$ and we find for c_1, c_2:

$$\epsilon_2=E_0\sqrt{2} \qquad \rightarrow$$

$$\boxed{c_1=\frac{1}{\sqrt{2(2-\sqrt{2})}}, \qquad c_2=\frac{\sqrt{2}-1}{\sqrt{2(2-\sqrt{2})}}}$$

Now that we have find the coefficients c_1, c_2 for the $\epsilon_2=E_0\sqrt{2}$ eigenvalue we repeat the exact same procedure for the eigenvalue $\epsilon_1=-E_0\sqrt{}$, (which obviously will lead to different c_1, c_2). Doing all these, the two eigenstates/eigenvalues, $|\phi_1\rangle, |\phi_2\rangle$ expressed in terms of the fundamental basis, [32] :

$$|\phi_1\rangle=\sqrt{\frac{1}{2(2+\sqrt{2})}}\begin{pmatrix}1\\-(\sqrt{2}+1)\end{pmatrix}, \qquad \epsilon_1=-E_0\sqrt{2},, \qquad (2.46)$$

$$|\phi_2\rangle=\sqrt{\frac{1}{2(2-\sqrt{2})}}\begin{pmatrix}1\\\sqrt{2}-1\end{pmatrix}, \qquad \epsilon_2=+E_0\sqrt{2}, \qquad (2.47)$$

Or re-expressed explicitly on the kets $|1\rangle, |2\rangle$:

$$|\phi_1\rangle=\sqrt{\frac{1}{2(2+\sqrt{2})}}\Big(|1\rangle-(\sqrt{2}+1)|2\rangle\Big), \qquad (2.48)$$

$$|\phi_2\rangle=\sqrt{\frac{1}{2(2-\sqrt{2})}}\Big(|1\rangle+(\sqrt{2}-1)|2\rangle\Big) \qquad (2.49)$$

b *Measurement of energy*. We know the system is at state $|1\rangle$. Since the results of an energy measurement are required we need to expand this state on the Hamiltonian's eigenbasis and interpret the expansion coefficients according to measurement postulate (QM3). From (2.48)-(2.49) it is straightforward to find:

$$|1\rangle=\left(\frac{1}{2}\sqrt{2-\sqrt{2}}\right)|\phi_1\rangle+\left(\frac{1}{2}\sqrt{2+\sqrt{2}}\right)|\phi_2\rangle \qquad (2.50)$$

$$|2\rangle=\left(-\frac{1}{2}\sqrt{2+\sqrt{2}}\right)|\phi_1\rangle+\left(\frac{1}{2}\sqrt{2-\sqrt{2}}\right)|\phi_2\rangle. \qquad (2.51)$$

So, at this point we have expanded the system's state $|1\rangle$ onto the Hamiltonian's eigenbasis according to (QM3). Since the eigestate $|\phi_1\rangle$ has as an eigenvalue $\epsilon_1=-E_0\sqrt{2}$ an energy measurement will give this value with probability,

$$P_1(E=-\frac{E_0}{\sqrt{2}})=|c_1|^2=\left|\frac{1}{2}\sqrt{2-\sqrt{2}}\right|^2=\frac{2-\sqrt{2}}{4},$$

32: One can easily check that these states are orthonormalized and that:

$$\hat{H}|\phi_1\rangle=-E_0\sqrt{2}|\phi_1\rangle$$
$$\hat{H}|\phi_2\rangle=E_0\sqrt{2}|\phi_2\rangle$$

and that,

$$\langle\phi_1|\phi_1\rangle=\langle\phi_2|\phi_2\rangle=1,$$
$$\langle\phi_1|\phi_2\rangle=\langle\phi_2|\phi_1\rangle=0$$

Note: The above solution is re-written as,

$$P_1(E<0)=\frac{2-\sqrt{2}}{4}=\frac{(\sqrt{2}-1)}{2\sqrt{2}}=\frac{(\sqrt{2}-1)(\sqrt{2}-1)}{2\sqrt{2}(\sqrt{2}-1)}=\frac{1}{2}\frac{(1-\sqrt{2})^2}{(2-\sqrt{2})}$$

Question 2.7.6

A system is in the state $|\psi\rangle$ of an N-dimensional space spanned by the eigenvectors of an arbitrary observable, $\hat{Q}$.

(a) Assume the state $|\psi\rangle$ written as a superposition of the $\hat{O}$ observable eigenbasis, $|q_n\rangle$:

$$|\psi\rangle=\sum_n c_n|q_n\rangle \qquad \rightarrow \qquad c_n=\langle q_n|\psi_n\rangle$$

(b) If $\mathbb{1}$ is the unit matrix, show that

$$\sum_n |q_n\rangle\langle q_n|=\mathbb{1}$$

The above relation hold in general or any eigenbasis of an observable and it is known as the *completeness* relation.

(c) A measurement of this observable provides the eigenvalue q_1 with probability p_1. If the system is instead in the state

$$|\psi'\rangle=e^{\imath\pi/2}|\psi\rangle$$

upon measurement of $\hat{Q}$ with what probability will provide the eigenvalue q_1?

Solution: (a) From the question and the QM1/QM2 postulates we have for the eigenbasis

$$\langle q_m|q_n\rangle=\delta_{mn}=\begin{cases}1 & n=m\\ 0 & n\neq m\end{cases}$$

Then by taking the inner product of the state $|\psi\rangle$ with an arbitrary eigenstate $|q_m\rangle$ we have,

$$\begin{aligned}\langle q_m||\psi\rangle\rangle&=\sum_n c_n\langle q_m|q_n\rangle=\sum_n c_n\delta_{nm}\\ &=c_1\times 0+c_2\times 0+\cdots+c_m\times 1+\cdots c_N\times 0=c_m\end{aligned}$$

Since m is arbitrary it holds for every $m=1,2,\cdots$ that

$$c_n=\langle q_n|\psi_n\rangle$$

(b)

From QM3 we have that a measurement of $\hat{Q}$ will give as an outcome

the eigenvalue q_1 with probability:

$$P_1(\hat{Q} = q_1) = |c_1|^2.$$

To find the probability to appear this same value q_1 of the observable $\hat{Q}$ when the system is in the state $|\psi'\rangle$ instead, we again expand on the same eigenbasis of $\hat{Q}$ as below:

$$|\psi'\rangle = e^{\imath\phi}|\psi\rangle = e^{\imath\phi}\sum_n c_n|q_n\rangle = \sum_n \left(e^{\imath\phi}c_n\right)|q_n\rangle = \sum_i C_n|q_n\rangle.$$

In our case, we set $\phi = \pi/2$. Therefore we have the expansion of $|\psi'\rangle$ on the eigenstate basis of $\hat{Q}$:

$$|\psi'\rangle = \sum_i C_i|q_i\rangle, \qquad \text{where} \qquad C_i = e^{\imath\phi}c_i.$$

Again, according to QM postulate (QM3), a measurement of $\hat{Q}$ will give the eigenvalue q_1 (associated with the eigenstate $|q_1\rangle$) with probability [33]:

$$P_{\psi'}(\hat{Q} = q_1) = |C_1|^2 = |e^{\imath\phi}c_1|^2 = |c_1|^2 = p_1 = P_{\psi}(\hat{Q} = q_1)$$

So eventually:

$$\boxed{P_{\psi'}(\hat{Q} = q_1) = P_{\psi}(\hat{Q} = q_1)}$$

From these we see that the measurements for all $P(\mathbb{Q} = q_n)$ probabilities remain the same regardless the value of ϕ. *This is to emphasize, once more, that for QM the states $|\psi\rangle$ and $e^{\imath\phi}|\psi\rangle$ represent the same physical state.*.

33: The symbol $P_{\psi'}(\hat{Q} = q_n)$ should be interpreted as:
the probability that the quantum system in state $|\psi\rangle$, upon a measurement of the observable $\hat{Q}$ will give the value q_n.

2.8 Some conclusive comments

So far, the discussion has been exclusively referred to a formulation of the quantum mechanics with the physical states as elements of an abstract Hilbert space. In the case of familiar 3D space vectors[34], the choice of a particular coordinate system, say $\mathscr{C}$ provides the means for the practical calculations turning abstract vector relation (as is for example the 2-nd Newton's law) to down-to-earth numerical relations between physical quantities. Translation and/or rotation of the coordinate system ($\mathscr{C} \rightarrow \mathscr{C}'$) transforms the original set of component, expressed in $\mathscr{C}$), in a controlled way, to another set of components (expressed now in $\mathscr{C}'$)[35]. The choice of the coordinate systems can greatly facilitate (or not) the numerical computations. Even more, the proper choice can offer an improved insight about the process under question or it can obscure it all. Recall the calculation of the electrostatic potential of a motionless uniformly charged spherical ball; one faces the choice between a spherical and Cartesian coordinate systems. What would be the wiser choice? [36] It seems that the identification of physical symmetries, possessed by the system, is a fairly reasonable starting point to choose a suitable coordinate system.

Having said the above one should realize that these lines of thinking are valid in quantum mechanical problems as well. The key idea is that quantum physical states (and operators) live in linear vector spaces and dealing with quantum mechanical systems, more often than not, a suitable eigenbasis set must be chosen to perform calculations. The eigenbasis set, used to expand the abstract vectors, corresponds to the (spatial) coordinate system of classical mechanics. It is hoped that the reader is now at a position that can see this analogy. Also, often the basis is dictated by the observable ($\mathbb{Q}$) under question and the type of the measurement to be performed and not only the system itself. Fortunately, the quantum observables via the eigenvalue equation generate an eigenbasis set. Picking the right observable and solving the eigenvalue equation is a step that one needs to go through in most cases. In the next chapter more applications of the fundamental QM principles will be discussed and applied to simple (and low dimension) quantum systems.

34: You may imagine for example the vectors representing the position, momentum and angular momentum of a particle, or the force acting on the particle.

35: Of course the relations between the involved set of components remain as dictated by the Physics laws. For example for a particle of mass m subject to a force governed by the Newton's 2nd law the ratio between acceleration and force still will be equal to particle's mass regardless what coordinate system happens to be in use ($\mathscr{C}$) or $\mathscr{C}'$

36: It turns to be the spherical in case you wonder. To appreciate this you may try to solve this problem in both coordinate systems

Measurement and Time Evolution of a state

3

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In this chapter the QM principles will be discussed in further detail and will be applied in the case of simple quantum systems such as spin, angular momentum and photon's polarization (prior to have discussed its actual physical nature). So let's summarize in the below a rather general scenario about various processes possible within QM theory.

So, lets take a physical system, S, and try to treat its properties within the QM theory. A certain, well chosen, particular properties of the system may be used to fully characterize the system uniquely. Such characterization maybe used to understand the inner workings of the system (often not accessible to observation) and eventually to allow the control of various physical processes at will. These properties could be, for example, position, momentum (linear and angular), energy, spin, etc, and in general any combination that could come out from simpler physical quantities and may suit our experimental equipment. [38]. These quantities (in QM are called observables, QM2) in general are *dynamic* that is, are varying in time. Consequently, in the case of measurements their values may change in time.

Measurement of observable $\hat{Q}$ when the system S is in state $|\psi\rangle$. Let's for the sake of clarity name the observable, $\hat{Q}$ and assume the state is in state $|\psi\rangle$. According to QM the state $|\psi\rangle$ can be expressed (linear superposition) in terms of any legitimate (orthonormal) vector basis, in the exact same sense that a physical position vector can be expanded on any orthonormal reference system $(\hat{x}, \hat{y}, \hat{z})$ suits us. Also according the QM each observable is associated with such basis, say $|q_n\rangle$, which can be calculated by recalling its *eigenvalue equation*:

$$\hat{Q}|q_n\rangle = \lambda_n|q_n\rangle \qquad \rightarrow \qquad (\ \lambda_n,\ \ |q_n\rangle\ ), \quad n = 1, 2, \cdots, N \tag{3.1}$$

Given the above, we may write for $|\psi\rangle$:

$$|\psi\rangle = \sum_n c_n|q_n\rangle. \tag{3.2}$$

The above is one among the possible expansions of the system's state, $|\psi\rangle$. It is the expansion on the eigenstates of $\hat{Q}$. This is required if we want to study the measurement results performed on the system as concerns the observable $\hat{Q}$.

So, we now know that *measurements* in QM give results of probabilistic nature, in the sense that the outcome has a probability to appear (QM3). More specifically if we perform a measurement of $\hat{Q}$ we'll obtain as a result anyone of the λ_n with probability $P(Q = \lambda_n) = |c_n|^2$ (To repeat

38: For example angular momentum is an example of such combination, $\mathbf{L} = \mathbf{r} \times \mathbf{p}$, where $\mathbf{r}, \mathbf{p}$ are the position and momentum of a quantum particle. Same reasoning for the kinetic energy, which its classical mechanics expressions is $p^2/2m$

here that this is known as the 'Born' rule).

$$|\psi\rangle \xrightarrow{\text{Measurement of } \hat{Q}} \lambda_n \quad \textit{with probability } |c_n|^2 \textit{ and system left in state } |q_n\rangle.$$

Also following the measurement of an observable which resulted to a particular eigenvalue, the state of the system is the eigenstate associated with the eigenvalue observed. The only exception to the latter is when the system is in one of the eigenstates of the observable being measured; then the measurement will give with certainty the eigenvalue associated with the particular eigenstate of the observable. In this case the above measurement scheme specializes to:

$$|q_n\rangle \xrightarrow{\text{Measurement of } \hat{Q}} \lambda_n \quad \textit{with probability } 1 \textit{ and system remains in state } |q_n\rangle\ .$$

Since the measurements provide random results it is reasonable to introduce some measures which provide useful information about the statistical properties of the quantity. Most useful are the average and the standard deviation of the $\hat{Q}$ measurements, given by,

$$\langle\hat{Q}\rangle = \sum_n q_n P(q_n), \qquad \Delta\hat{Q} = \sqrt{\langle\left(\hat{Q} - \langle Q\rangle\right)^2\rangle} = \sqrt{\langle\hat{Q}^2\rangle - \langle\hat{Q}\rangle^2} \tag{3.3}$$

QM provides the following expression for the (quantum) average (or expectation value):

$$\langle Q\rangle_\psi = \langle\psi|\hat{Q}|\psi\rangle \tag{3.4}$$

where the above expression should be understood as a row-vector by matrix by column-vector calculation, since in QM $\langle\psi|$ in a $N \times N$ basis are $1 \times N$ row-vectors, operators are matrices and the ket $|\psi\rangle$ are $N \times 1$ column-vectors.

One may ask here, is there any advantage of (3.4) over (3.3)? The answer is affirmative; Expression (3.4) is more general than 3.3); the former is an expression independent on any particular basis states, $|q_n\rangle$ while the latter not. To understand the difference one can take the example of kinetic energy in classical mechanics. Assuming a particle moving with velocity **v** its expression in terms of the vector **v** is given by,

$$T = \frac{1}{2}m\mathbf{v}^2.$$

Now, assuming that we work on a particular coordinate system (or reference frame), say, $Oxyz$, where the vector has components (v_x, v_y, v_z) we can also calculate its kinetic energy by means of these components:

$$T = \frac{1}{2}m(v_x^2 + v_y^2 + v_z^2).$$

However, this calculation is specific to the chosen reference frame. Had we chosen a different one (i.e. by rotating by a certain angle abound one the $Oxyz$ axes) then we have a new one, say $O\hat{x}'\hat{y}'\hat{z}'$ then the expression for the kinetic energy to calculate it would have changed to

$$T = \frac{1}{2}m\left[(v_x')^2 + (v_y')^2 + (v_z')^2\right].$$

Obviously, the kinetic energy found is using any of these three expres-

sions should be the same since the magnitude of **v** (length) doesn't change, simply because we changed the coordinate system.

This is exactly the situation between (3.4) over (3.3). The former is the 'vector' analogy of $T = \frac{1}{2}m\mathbf{v}^2$. it's the quantum average expression with no reference to any particular basis; the latter one is the quantum expression for the quantum average $\langle\hat{Q}\rangle$, *when the* $|\psi\rangle$ *vector and* $\hat{Q}$ *matrix are expressed on the eigenbasis of* $\hat{Q}$. Obviously, the general expression is preferred, since we may have $|\psi\rangle$ and $\hat{Q}$ expressed to any arbitrary basis, other than the $\hat{Q}$ eigenbasis.

One reasonable question (and more than often encountered) is how we work when we have the state expanded in the basis of $\hat{Q}$ as in (3.2) and then we ask the results of measurements of another observable, say $\hat{Q}'$. For example: We may have the state expanded on its Hamiltonian basis (Energy observable) and ask for the results of spin-measurements; or we may have the state expanded on the eigenstates of the $\hat{S}_z$ spin observable and then we ask the results of measurements of the $\hat{S}_x$ (or $\hat{S}_y$) observable. How we work in this case? The most straightforward way to go is the following:

(a) we solve again the eigenvalue problem of $\hat{Q}'$ and evaluate its eigenvalues, λ'_n and its associated eigenstates $|q'_n\rangle$

(b) Then we relate the q_n-basis with the q'_n-basis.

(c) From (b) we turn $|\psi\rangle = \sum_n c_n|q_n\rangle \rightarrow |\psi\rangle = \sum_n c'_n|q'_n\rangle$

(d) From this point on we work as usual to get probabilities and averages for $\hat{Q}'$ measurements since our state is expanded in terms of the $\hat{Q}'$ observable's eigenbasis, $|q'_n\rangle$.

However, if we had to evaluate either the quantum average, $\langle\hat{Q}'\rangle_\psi$ and/or its standard deviation $\Delta\hat{Q}'_\psi$ then we don't need to go through (a)-(d) above; we simply use the expression (3.4) for the averages, since this one applies regardeless the eigenbasis on which the states and the observables are represented.

Measurement's uncertainty and commutation relations

From the very nature of QM theory we know that measurement results (of an arbitrary observable, $\hat{Q}$) are of probabilistic nature and therefore, in the general case, there is an associated uncertainty which is inherent; QM provides no more help, beyond the probability of appearance of an outcome (which as we now know should be among the eigenvalues of $\hat{Q}$). Nevertheless we also know that if the measurement gives one of the eigenvalue, say λ_n, then the system is in the corresponding eigenvalue, $|q_n\rangle$. All these related by the eigenvalue equation,

$$\hat{Q}|q_n\rangle = \lambda_n|q_n\rangle.$$

So, if the system is in the state $|q_n\rangle$ this means that a second measurement will give the value of λ_n with certainty. However we know that a system is not characterized by just one observable [39] but, generally for more than one. A concrete example is the following: Assume the

39: For example an electron can be characterized by measurements of its position, velocity, energy, linear momentum, angular momentum, spin and so on.

spin state of an electron in an atomic orbital. The spin is an observable which has direction and magnitude; Assuming the spin as a classical quantity is written,

$$\mathbf{S} = \hat{x}S_x + \hat{y}S_y + \hat{z}S_z$$

As a classical quantity, then a complete characterization of the spin would require to measure all three S_x, S_y, S_z, along the three possible directions in space and then the spin $\mathbf{S}$ is completely known. This means that we can perform a measurement of S_x *without affecting the electron's state* and as a sequence does not affect the results of measurement of S_y and S_z. Unfortunately, this is not, in general, the case in QM; we know by QM3 that a measurement of $|\psi\rangle$ does change unpredictably the system's state bringing into one of the eigenstates of the measured observable, $|q_n\rangle$. It is then reasonable to conclude that this particular property has a consequence that not all observables can measured in an independent fashion. So a question arises whether one can go deeper to analyzing the statistical predictions of measurement results of two different observables, say $\hat{A}$ and $\hat{B}$.[40]

In the below, we give a general statement which hold for any such arbitrary observables. It is presented here without proof since the derivation is purely mathematical and no any particular (physical) requirements are invoked. So emphasizing on the final expression, the mathematical considerations for the QM's observables result to the following relation:

Uncertainty relation

$$(\Delta\hat{A})_\psi(\Delta\hat{B})_\psi \geq \frac{1}{2}\left|\langle\Psi|\left[\hat{A},\hat{B}\right]|\Psi\rangle\right|. \tag{3.5}$$

where $(\Delta\hat{A})_\psi$, $(\Delta\hat{B})_\psi$ are the corresponding uncertainties in the measurements of $\hat{A}$ and $\hat{B}$. [41]

The above expression is known as *uncertainty relations* [42] and give a prominence role on the commutator of the two observables. Let's see what one can conclude from the above. The possible measurement outcomes are the eigenvalues of the observables; these values satisfy the corresponding eigenvalue equations:

$$\hat{A}|A_n\rangle = a_n|A_n\rangle$$
$$\hat{B}|B_n\rangle = b_n|B_n\rangle.$$

Assume now we measure, say $\hat{A}$, and get one of its eigenvalues, say a_n. Then the system will be in the state $|A_n\rangle$. In this state the uncertainty of $\hat{A}$ will be zero $(\Delta\hat{A})_{a_n} = 0$ (since the state is an eigenstate of $\hat{A}$ and any subsequent measurement will give a_n with certainty. So $\langle A\rangle = a_n$ and $(\Delta A)_{a_n} = 0$).

At this point conclusions are different depending on whether the commutator $[\hat{A},\hat{B}]$ vanishes or not. So we separate the cases:

40: In the particular example of the spin, QM predicts that one can measure only, S^2 and one of its components, $\hat{S}_x$ or $\hat{S}_y$, or $\hat{S}_z$. It is not possible to have measurements of the components without these measurements affecting each other. In other words, measurement of $\hat{S}_z$ will affect the measurement results for $\hat{S}_x$ and $\hat{S}_y$ and vice versa.

41: The combination $\hat{A}\hat{B} - \hat{B}\hat{A}$ is known as *commutator* of $\hat{A}$ and $\hat{B}$

$$\left[\hat{A},\hat{B}\right] = \hat{A}\hat{B} - \hat{B}\hat{A}. \tag{3.6}$$

Note here that the order of the operators matters. You may think of this operation as matrix multiplication. Matrix multiplication is not a commutative operation. Also note that one can easily see that,

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

42: When applied to position and momentum, $\hat{A} = \hat{r}$ and $\hat{B} = \hat{p}$ we'll see that will result to,

$$[\hat{r},\hat{p}] = \imath\hbar,$$

The above three relations (3 for each component) were first derived by Heisenberg at 1925 and are generally known as Heisenberg relations.

$[\hat{A}, \hat{B}] \neq 0$. Now if $|\langle[\hat{A}, \hat{B}]\rangle| = |\langle\hat{A}\hat{B} - \hat{B}\hat{A}\rangle| = K \neq 0$, we have,

$$(\Delta\hat{A})_\psi(\Delta\hat{B})_\psi \geq K, \qquad K \text{ a real positive number.}$$

However, if instead try to measure $\hat{B}$, the above relation must be satisfied by measurements of $\hat{B}$:

$$(\Delta\hat{A})_{a_n}(\Delta\hat{B})_{a_n} = 0 \cdot (\Delta\hat{B})_{a_n} \geq K.$$

The above can only be fulfilled if $(\Delta\hat{B})_{a_n} = \infty$ (since any finite value which in practice means that our measurement is completely unpredictable! Then it is not possible to have knowledge of the measurement of $\hat{A}$ and $\hat{B}$ at the same time. Because, if we proceed with a measurement with $\hat{B}$ which result to, say b_n, the system's state will be $|B_n\rangle$ and then will have $\Delta B_n = 0$. But, following the same argument as before the Heiseberg relation would be fulfilled only if $((\Delta A)_{b_n} = \infty)$, so any predictability has been destroyed now! We then say the the observables, $\hat{A}$ and $\hat{B}$ are *incompatible*

$[\hat{A}, \hat{B}] = 0$. First we should note that in this case $\hat{A}$ and $\hat{B}$ have a common set of eigenstates but with *different eigenvalues*. So by setting, $|A_n\rangle = |B_n\rangle = |\phi_n\rangle$ we may write,

$$\begin{aligned} [\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} = 0 \quad \rightarrow \\ \hat{A}|\phi_n\rangle = a_n|\phi_n\rangle \\ \hat{B}|\phi_n\rangle = b_n|\phi_n\rangle. \end{aligned}$$

The above means that following the measurement of $\hat{A}$ which gives, say a_n, the state will then be ϕ_n. But this is an eigenstate of $\hat{B}$ as well, so a subsequent measurement of $\hat{B}$ will give with certainty b_n! In other words we are in a state of the system where a measurement of $\hat{A}$ and $\hat{B}$ will give a_n and b_n with certainty. We then say the the observables, $\hat{A}$ and $\hat{B}$ are *compatible*.

3.1 Dynamics when the system S is in state $|\psi\rangle$.

On the other hand, *if we allow the system unperturbed*, generally it is expected that its properties will change over time; the system S evolves. So in the general case the state $|\psi(t)\rangle$ [43] will change and as a result any measurement of any arbitrary observable $\hat{Q}$ at a later (or earlier) time than t will provide different values. Again to emphasize, in the general case; there some special states, which if the system found at a particular time, then its properties will not change over time; these are the so-called (for this reason) *stationary* states and are the eigenstates of the system's energy observable, with the corresponding operator known as *Hamiltonian*. In any case, the way to proceed is to calculate the evolution of $|\psi(t)\rangle$; this is the role of the time-dependent Schrödinger equation (TDSE), which is a deterministic law (in complete contrast with the probabilistic measurement 'law'); The meaning of this statement is that if we know the state $|\psi(t)\rangle$ at any given time, t and provided that we can work out the TDSE then we know the system's state $|\psi(t')\rangle$ at any time t' with *certainty*.

43: Let's now introduce the time explicitly, so that have clarity about the instant that the system's state is considered

QM gives a key role in the system's Hamiltonian, $\hat{H}$, in the sense that it's action on the system's states causes a time-shift of the state (forward or backward in time); this is expressed via the TDSE for the ket state, $|\psi(t)\rangle$

TDSE for the state's ket

$$\imath\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle, \qquad |\psi_0\rangle \equiv |\psi(t_0)\rangle, \tag{3.7}$$

From the above it's easy to see how the state is time-shifted when the Hamiltonian operator is acting on $|\psi(t)\rangle$. By definition of a derivative as $\dot{f} = df/dt$, use of (2.36) we take:

$$d|\psi\rangle = -\frac{\imath}{\hbar}dt\hat{H}|\psi(t)\rangle \qquad \rightarrow \qquad |\psi(t+dt\rangle - |\psi(t)\rangle = -\frac{\imath}{\hbar}dt\hat{H}(t)|\psi(t)\rangle$$

and finally we have the alternative expression (and fully equivalent to the TDSE)

Time shifted state

$$|\psi(t+dt\rangle = |\psi(t)\rangle - \frac{\imath}{\hbar}dt\hat{H}(t)|\psi(t)\rangle \tag{3.8}$$

Before we proceed further a need to complete the discussion of the TDSE is required. Expression (3.7) is a time-evolution law (basis-independent) for the system's ket $|\psi(t)\rangle$ state; but what about the system's bra $\langle\psi(t)|$? Of course there is a corresponding TDSE law and this can be derived by taking the complex-conjugate of the TDSE (3.7)

expression [44] :

$$\left(\imath\hbar\frac{\partial}{\partial t}|\psi(t)\rangle\right)^\dagger = \left(\hat{H}(t)|\psi(t)\rangle\right)^\dagger \qquad \rightarrow \qquad -\imath\hbar\frac{\partial}{\partial t}\langle\psi(t)| = \langle\psi(t)|\hat{H}^\dagger(t),$$

where we have taken into account that for any product between matrices or matrix-vector we have, $(AB)^\dagger = B^\dagger A^\dagger$. Now taking into account that all observables in QM are hermitian (which for us means, $\hat{H}^\dagger = \hat{H}$ we arrive to the following alternative TDSE expression for the state's bra:

TDSE for the state's bra

$$-\imath\hbar\frac{\partial}{\partial t}\langle\psi(t)| = \langle\psi(t)|\hat{H}(t), \qquad \langle\psi_0| \equiv \langle\psi(t_0)|, \tag{3.9}$$

To have an idea how the TDSEs for the state's bra and ket look like in practice let's take the case of a state of dimension 2 (say, electronic's spin state) in some orthonormalized basis, represented by the fundamental basis $|v_1\rangle = \begin{pmatrix}1\\0\end{pmatrix}$ and $|v_2\rangle = \begin{pmatrix}0\\1\end{pmatrix}$. Then assuming the representations of $|\psi\rangle$ and $\hat{H}$ on this basis, by

$$|\psi(t)\rangle = \begin{pmatrix}c_1\\c_2\end{pmatrix}, \quad \langle\psi(t)| = \begin{pmatrix}c_1^\star, c_2^\star\end{pmatrix}, \qquad \hat{H}(t) = \begin{pmatrix}h_{11}(t) & h_{12}(t)\\ h_{12}^\star(t) & h_{22}(t)\end{pmatrix},$$

where, $c_i = c_i(t),\ i = 1,2$ and $h_{ij} = h_{ij}(t)$ are generally complex time-dependent numbers. the TDSEs (3.7) would be expressed as,

$$\imath\hbar\frac{d}{dt}\underbrace{\begin{pmatrix}c_1(t)\\c_2(t)\end{pmatrix}}_{|\psi(t)\rangle} = \underbrace{\begin{pmatrix}h_{11} & h_{12}\\ h_{12}^\star & h_{22}\end{pmatrix}}_{\hat{H}(t)}\underbrace{\begin{pmatrix}c_1(t)\\c_2(t)\end{pmatrix}}_{|\psi(t)\rangle} \tag{3.10}$$

and for the (3.9) as,[45]

$$-\imath\hbar\frac{d}{dt}\underbrace{\left(c_1^\star(t), c_2^\star(t)\right)}_{\langle\psi(t)|} = \underbrace{\left(c_1^\star(t), c_2^\star(t)\right)}_{\langle\psi(t)|}\underbrace{\begin{pmatrix}h_{11} & h_{12}\\ h_{12}^\star & h_{22}\end{pmatrix}}_{\hat{H}(t)} \tag{3.11}$$

It should obvious now that the Hamiltonian plays a very important role in QM, not unexpectedly as in classical physics the energy of a system is an important concept. For example, by definition, an isolated mechanical system has its energy constant, that is the sum of the kinetic energy of its constituents and the potential energy,

$$E = \sum_i \frac{1}{2}\mathbf{v}_i^2 + U(\mathbf{r}_i) = \text{const.}$$

This a known property of this quantity, provided the potential energy is not explicitly time-dependent. [46] So, it looks like that the corresponding observable in QM, the Hamiltonian operator, keeps its dominant role when characterizing a quantum system. Eventually it is proven worth

44: Taking the 'dagger' of a number, vector or matrix consists of the followings:

- For number just take its complex conjugate $(a+\imath b)^\dagger \rightarrow (a-\imath b)$
$$(\imath)^\dagger = -\imath$$
- If it is column-vector then take its row-vector and then its complex-conjugate. If it's row-vector, take its column-vector and then its complex-conjugate. This means,
$$(|\psi\rangle)^\dagger = \langle\psi|, \qquad (\langle\psi|)^\dagger = |\psi\rangle$$
Example for $|\psi\rangle = \begin{pmatrix}a\\b\end{pmatrix}$ and $\boldsymbol{\phi} = \begin{pmatrix}c, d\end{pmatrix}$:
$$(|\psi\rangle)^\dagger = \begin{pmatrix}a\\b\end{pmatrix}^\dagger = \begin{pmatrix}a^\star, b^\star\end{pmatrix}$$
and
$$(|\phi\rangle)^\dagger = \begin{pmatrix}c, d\end{pmatrix}^\dagger = \begin{pmatrix}c^\star\\d^\star\end{pmatrix}$$
- If it is matrix, take its transpose and then its complex conjugate. Example:
$$\begin{pmatrix}a & b\\ c & d\end{pmatrix}^\dagger = \begin{pmatrix}a^\star & c^\star\\ c^\star & d^\star\end{pmatrix}$$

Note that the usual properties of the matrix algebra hold here as well. So for the 'dagger' of a product of matrices we have,
$$(AB)^\dagger = B^\dagger A^\dagger$$

45:

Question 3.1.1

Can you write down the expression for the bra $\langle\psi(t+\tau)|$ corresponding to Eq. (3.8)?

46: When it is time-dependent, the total energy it is still an important quantity in classical mechanics, nevertheless it is not constant of the motion, anymore.

to explore the dynamics of a QS when its Hamiltonian operator is not explicitly time dependent. This is the subject of the next section. We'll see that keeping track of the time-evolution properties of the system simplifies to a large degree.

3.2 Quantum dynamics under a constant Hamiltonian.

The assumption of a Hamiltonian operator which does not depend explicitly on time is mathematically expressed by,

$$\frac{d\hat{H}}{dt} = 0. \tag{3.12}$$

Our task in this section is the following:

Given that state known at some instant, say, t_0 what is the system's state at time t?

Mathematically this is also expressed as,

$$\text{If} \quad |\psi(t_0)\rangle \quad \text{known, then} \quad |\psi(t)\rangle = ?$$

Why this is required? Simply because that anything that can be said for the system is contained in the state $|\psi(t)\rangle$. So by knowing this state we can then predict the measurement results of any observable $\hat{Q}$, following the standard procedure described in the last section.

So turning into the task of determining $|\psi(t)\rangle$ we notice that the fact that the Hamiltonian is 'constant-of-motion' necessarily means that the eigenvalue equation for the Hamiltonian will provide a time-independent eigenbasis set (eigenvalues and eigenstates). Given that this basis set can be used to expand the system's state we can investigate the dynamics on this particular basis. This is one of the approaches that one can use. The expressions derived will be basis-dependent.

Dynamics of $|\psi(t)\rangle$ on the Hamiltonian eigenbasis.

The eigenvalue equation for the Hamiltonian, also known as *time-independent Schrödinger Equation* (TISE) is, [47]

$$\hat{H}|E_n\rangle = E_n|E_n\rangle. \tag{3.13}$$

It is now straightforward to see that since the Hamiltonian operator energy doesn't change with time, the eigenvectors $|E\rangle$ (and eigenvalues, E_n) also don't change. So, following the standard procedure we expand our quantum state in terms of these eigenstates,

$$|\psi(t)\rangle = \sum_n c_n(t)|E_n\rangle, \tag{3.14}$$

where $c_n(t)$ represent the expansion coefficients on the energy eigenbasis (the equivalent of components in conventional vector algebra of 'physical' vectors such as positions and velocities.). With the eigenstates, $|E_n\rangle$ constants, it is concluded that all of the evolution of the quantum state has to be in the coefficients expansions, $c_n(t)$.

47: The notation we used so far to express an eigenvalue problem for an observable would have been call for,

$$\hat{H}\,|q_n\rangle = \lambda_n\,|q_n\rangle.$$

But for more clarity it's better to choose a notation which declares explicitly which operator's the eigenvalues/eigenstates stand for. So we adapt accordingly the notation by:

$$|q_n\rangle \to |E\rangle, \quad \lambda_n \to E_n$$

The expansion (3.14) is used with conjunction to the TDSE to determine the $c_n(t)$ coefficients:

$$\begin{aligned}
\imath\hbar\frac{d}{dt}|\psi(t)\rangle &= \hat{H}|\psi(t)\rangle \\
\downarrow \qquad & \qquad \downarrow \\
\imath\hbar\frac{d}{dt}\left[\sum_n c_n(t)|E_n\rangle\right] &= \hat{H}\left[\sum_n c_n(t)|E_n\rangle\right] \\
\downarrow \qquad & \qquad \downarrow \\
\imath\hbar\sum_n \frac{dc_n(t)}{dt}|E_n\rangle &= \sum_n c_n(t)\hat{H}|E_n\rangle = \sum_n c_n(t)E_n|E_n\rangle,
\end{aligned}$$

where in the last equality we used the TISE (3.13) So, re-arranging everything on the same side,

$$\sum_n \left[\imath\hbar\frac{dc_n(t)}{dt} - E_n c_n(t)\right]|E_n\rangle = 0. \tag{3.15}$$

The left-hand-side is zero only if every term in the square brackets is zero (since $|E_n\rangle$ cannot be *all* zero):

$$\imath\hbar\frac{dc_n(t)}{dt} = E_n c_n(t). \tag{3.16}$$

For a specific solution of the above first-order ordinary differential equation (ODE) we need an initial condition for the coefficients. This is obtained by evaluating the initial state at time t_0:

$$|\psi(t_0)\rangle = \sum_n c_n(t_0)|E_n\rangle \qquad \rightarrow \qquad \text{all } c_n(t_0) \text{ assumed known.}$$

With this initial condition we arrive to the solution [48] ,

$$c_n(t) = c_n(0)e^{-\frac{\imath}{\hbar}E_n t}, \tag{3.17}$$

Eventually, when the Hamiltonian is time-independent, we arrive at the following simple expression for the evolved state, $|\psi(t)\rangle$ [49]

$$|\psi(t)\rangle = \sum_n c_n(t_0)e^{-\frac{\imath}{\hbar}E_n(t-t_0)}|E_n\rangle. \tag{3.18}$$

It is then concluded that in the energy eigenbasis we only require knowledge of the expansion coefficients at a particular time, namely knowledge of $c_n(t_0)$.

Summarizing all the above the steps required to calculate the time evolution of a state known at time t_0, namely, with $|psi(t_0)\rangle$ known:

Calculation of the state $|\psi(t)\rangle$ in the energy basis.

(i) Identify $\hat{H}$.
(ii) Find the eigenvalues E_n and eigenvectors $|E_n\rangle$ of the Hamil-

48: The ODE is with constant coefficient and it is easily solved as, by simple re-arrangement of (3.16),

$$\begin{aligned}
&\rightarrow \frac{dc_n}{c_n} = -\frac{\imath}{\hbar}E_n dt \\
&\rightarrow \int_{c_n(t_0)}^{c_n(t)} \frac{dc_n'}{c_n'} = -\frac{\imath}{\hbar}\int_{t_0}^{t} E_n dt' \\
&\rightarrow \ln c_n(t) - \ln c_n(t_0) = -\frac{\imath}{\hbar}(t-t_0) \\
&\rightarrow \ln\frac{c_n(t)}{c_n(t_0)} = -\frac{\imath}{\hbar}(t-t_0).
\end{aligned}$$

Taking the exponent of the last equation we end up to (3.17).

49: Can you write the quickly the corresponding expression for the bra $\langle\psi(t)|$, provided you know either $||\psi(t_0)\rangle$ or $\langle\psi(t_0)|$?

tonian $\hat{H}$ by solving:

$$\hat{H}|E_n\rangle = E_n|E_n\rangle \tag{3.19}$$

(iii) Identify the instant, t_0, that the state is known and expand in terms of $|E_n\rangle$:

$$|\psi(t_0)\rangle = \sum_n c_n(0)|E_n\rangle. \tag{3.20}$$

Determine $c_n(0)$ from this expansion.

(iv) Then the state at time t is:

$$|\psi(t)\rangle = \sum_n c_n(0)e^{-\frac{\imath}{\hbar}E_n t}|E_n\rangle. \tag{3.21}$$

From this point on, we can proceed and calculate the results of measurements of any given arbitrary observable, $\hat{Q}$ following the QM principle for the measurement operation.

The time-evolution operator

Normally, our next task it would be to provide a solution for the state's time evolution which is *independent on any particular basis*. Certainly, such independence will make the solution amenable to investigating quantum processes and reach conclusions which are of general validity. Which method to use, depends on the problem under consideration. The basis-independent solution starts from repeated use of (3.8) which entails to the following basis-independent expression for $|\psi(t)\rangle$:

Evolution operator

$$|\psi(t)\rangle = e^{-\frac{\imath}{\hbar}\hat{H}(t-t_0)}|\psi(t_0)\rangle. \tag{3.22}$$

In the above, the exponentiation of the Hamiltonian operator is actually another operator (also represented by a matrix) known as the system's evolution operator,

$$\hat{U}(t,t_0) = e^{-\frac{\imath}{\hbar}\hat{H}(t-t_0)} \tag{3.23}$$

One may ask how one can evaluate the exponent of a matrix. This is done by use of the well-known Taylor series for ordinary numbers. [50] Therefore in analogy with the Taylor expansion we have a practical expression:

$$\hat{U}(t,t_0) = e^{-\frac{\imath}{\hbar}\hat{H}\tau} = \mathbb{1} - \frac{\imath}{\hbar}\tau\hat{H} - \frac{1}{\hbar^2}\hat{H}^2\tau^2 + \cdots, \quad \tau = t - t_0 \tag{3.24}$$

So, in practice, for a Hamiltonian where the time does not appear explicitly we have a very specific (and handy) rule to obtain the system's state $|\psi(t)\rangle$ given the $|\psi(t_0)\rangle$: Multiply the *evolution* matrix $U(t,t_0) = e^{-\frac{\imath}{\hbar}\hat{H}(t-t_0)}$ with the vector $|\psi(t_0)\rangle$ (representing the system's state at t_0) to get the state shifted at time t, later or earlier as $t > t_0$ or $t < t_0$.

50:

$$e^x = \sum_k \frac{x^n}{n!} = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots$$

Nevertheless, at this point we'll refrain from heavy use this more general solution until we have reached a certain level of familiarity with the present quantum formulation. So, at the moment we'll be treating quantum dynamics following the steps described in last section.

Question 3.2.1

Assume a state $|\psi(t_0)\rangle$ expanded on the energy eigenstates, $|E_n\rangle$ at time t_0. Using (3.22) show that $|\psi\rangle$ is expressed identically as in (3.21).

3.3 Time-evolution of quantum averages

Now that a basic theory to modeling the time evolution of a quantum state, we can ask the question what happens to measurable quantities as time evolves. More specifically, what happens to the average of a measurement over time? Let's start with an arbitrary observable $\hat{Q}(t)$. We also allow the general case where the observable may depend explicitly on time. As known, the expectation value is

$$\left\langle \hat{Q}(t) \right\rangle_{\psi} = \langle \psi(t) | \hat{Q} | \psi(t) \rangle. \tag{3.25}$$

The question is simple. The above expression is a number which is nothing else than the average value of the measurements of the observable, $\hat{Q}$. The question is as follows: if we let the state to evolve in time and perform the measurement at an arbitrary time what happen to $\left\langle \hat{Q} \right\rangle_{\psi}$? Does it change and how? To answer this question it helps to find a time-evolution law in analogy the TDSE law for the state $|\psi(t)\rangle$. Let's take the time derivative an use the product rule from ordinary calculus:

$$\begin{aligned}
&\frac{d}{dt}\left\langle \hat{Q} \right\rangle = \frac{d}{dt}\left[\langle \psi(t) | \cdot \hat{Q} \cdot | \psi(t) \rangle \right] = \\
&= \underbrace{\left[\frac{d}{dt} \langle \psi(t) | \right]}\, \hat{Q} | \psi(t) \rangle + \underbrace{\langle \psi(t) | \left(\frac{\partial}{\partial t} \hat{Q} \right) | \psi(t) \rangle}_{\langle \frac{\partial \hat{Q}}{\partial t} \rangle} + \langle \psi(t) | \hat{Q} \underbrace{\left[\frac{d}{dt} | \psi(t) \rangle \right]}. \\
&\frac{d}{dt} \langle \psi(t) | = \frac{\imath}{\hbar} \hat{H} \qquad\qquad \frac{d}{dt} | \psi(t) \rangle = -\frac{\imath}{\hbar} \hat{H}
\end{aligned}$$

We combine the two operator terms and write the middle term as an expectation value:

$$\begin{aligned}
\frac{d}{dt}\left\langle \hat{Q} \right\rangle &= \frac{\imath}{\hbar} \langle \psi(t) | \left[\hat{H}\hat{Q} - \hat{Q}\hat{H} \right] | \psi(t) \rangle + \left\langle \frac{\partial}{\partial t} \hat{Q} \right\rangle \\
&= \frac{\imath}{\hbar} \left\langle \left[\hat{H}, \hat{Q} \right] \right\rangle + \left\langle \frac{\partial}{\partial t} \hat{Q} \right\rangle,
\end{aligned}$$

where, $[\hat{H}, \hat{Q}] = \hat{H}\hat{Q} - \hat{Q}\hat{H}$. Eventually we arrive to the so-called Ehrefenst theorem for the expectation value:

Ehrenfest theorem

$$\imath\hbar \frac{d}{dt} \langle \hat{Q} \rangle_{\psi} = \langle [\hat{Q}, \hat{H}] \rangle_{\psi} + \imath\hbar \langle \frac{\partial \hat{Q}}{\partial t} \rangle_{\psi} \tag{3.26}$$

Conservation Laws for constant observables

Again, mathematically this is expressed by setting,

$$\frac{\partial \hat{Q}}{\partial t} = 0.$$

Under this assumption let's investigate a bit more closely what conclusions can be reached by using the Ehrenfest theorem as expressed in (3.26).

The energy observable, $\hat{Q} = \hat{H}$.

Then, since, $[\hat{H}, \hat{H}]$ is identically zero, we can immediately see that for any state $|\psi\rangle$ we have,

$$\imath\hbar \frac{d}{dt}\langle \hat{H}\rangle_\psi = \langle \left[\hat{H}, \hat{H}\right]\rangle_\psi = 0 \qquad \rightarrow \qquad \langle \hat{H}\rangle_\psi = E = \text{const.}$$

What the above result says is that the average value of energy of a system where its Hamiltonian does not explicitly contain time stays constant. In other words energy measurements will show no difference with the course of the time. Accordingly we can find that the energy uncertainty, $(\Delta\hat{H})_\psi$ is constant. We see then that the statistical properties of the measurement results remain constant. We can then say that the energy measurement results is a *stationary* random variable. Although, the state $|\psi(t)\rangle$ may vary in time, the corresponding averaged quantities do not change:

$$\langle \hat{H}\rangle_\psi = E = cnst. \qquad (\Delta\hat{H})_\psi = \Delta E = cnst$$

Observables which commute with the Hamiltonian, $[\hat{Q}, \hat{H}] = 0$ In this case we again reach the same conclusion as for the energy observable, namely that,

$$\imath\hbar \frac{d}{dt}\langle \hat{Q}\rangle_\psi = \langle \left[\hat{H}, \hat{Q}\right]\rangle_\psi = 0 \qquad \rightarrow \qquad \langle \hat{Q}\rangle_\psi = \text{const.}$$

We thus can see the importance of the commutation property with the Hamiltonian. If an arbitrary observable commutes with the Hamiltonian, that is,

$$\hat{Q}\hat{H} = \hat{H}\hat{Q}$$

then this observable also has an average value which is constant. The underlying reason for this is that in this case the $\hat{Q}$ observable has the same eigenstates as the Hamiltonian, $|E_n\rangle$ but associated with different eigenvalues, q_n. So the following property holds,[51]

$$[\hat{Q}, \hat{H}] = 0 \qquad \rightarrow \qquad \hat{Q}|E_n\rangle = q_n|E_n\rangle. \tag{3.27}$$

51: More generally, any two observables with commutator $[A, B] = 0$ share the same eigenstates set.

Characteristic time-evolution

Let's use now the Ehrenfest theorem for an alternative insight in the time evolution of quantum system. It makes sense to define a characteristic evolution time, which essentially will give as an idea how quickly a system change its properties relative to an arbitrary observable. We know now that this will be the case when $[\hat{Q}, \hat{H}] \neq 0$. Again, ignoring any explicit time dependence of the operator, we have

$$\frac{d}{dt}\left\langle \hat{Q}\right\rangle = \frac{\imath}{\hbar}\left\langle \left[\hat{H}, \hat{Q}\right]\right\rangle. \tag{3.28}$$

Let's define the characteristic time scale over which a noticeable change. However, we have first to define what we mean by 'noticeable' change here. The measurements outcomes of an observable have a probability distribution among the eigenvalues of the observable. So the results are random and has certain statistical properties. As discussed the most important are the average and the associated standard deviation (s.d.) (or uncertainty in QM terminology). The s.d. is a measure of the spread of the results around its average. Low s.d. means narrow spread around the average while high s.d. means a broad spread of the results around $\langle\hat{Q}\rangle$. So, if the average $\langle\hat{Q}\rangle$ is to change over time then a noticeable change would mean relative to its uncertainty (s.d.) value. Therefore we can ask the question: Given that the rate of change of $\langle\hat{Q}\rangle$ is equal to $R = |d\langle\hat{Q}\rangle|/dt$ then how long it takes to change by $(\Delta\hat{Q})$? If we name this time, τ_q, mathematically this is expressed as,

$$\Delta Q = R\tau_q \qquad \rightarrow \qquad \tau_q = \frac{\Delta Q}{R}.$$

But $R = |d\langle\hat{Q}\rangle|/dt$ is given by the Ehrenfest law to arrive at,

$$\tau_q \equiv \frac{(\Delta\hat{Q})_\psi}{\left|d\left\langle\hat{Q}\right\rangle/dt\right|} = \frac{\hbar(\Delta\hat{Q})_\psi}{\left|\langle[\hat{Q},\hat{H}]\rangle_\psi\right|} \tag{3.29}$$

where $(\Delta\hat{Q})_\psi$ is the measurement's uncertainty (s.d.) of the observable. In lay language, this means that it takes time Δt for the observable to change enough for us to be able to measure the change. Note that this characteristic time depends on the state, $|\psi(t)\rangle$ of the system, and therefore generally may vary in time.

Now we can make use of the general uncertainty relation (3.5) for the observable $\hat{Q}$ and $\hat{H}$. Setting, $(\Delta\hat{H})_\psi = \Delta E$ we have,

$$(\Delta\hat{Q})_\psi(\Delta E) \geq \frac{1}{2}\left|\langle\left[\hat{Q},\hat{H}\right]\rangle\right|.$$

But from (3.29) we have, $\left|\langle[\hat{Q},\hat{H}]\rangle_\psi\right| = \tau_q\hbar(\Delta\hat{Q})_\psi$ and we end to the following relationship:

$$\tau_q \geq \frac{\hbar}{2\Delta E}$$

The quantity $\tau_E = \hbar/2\Delta E$ has the dimensions of time and it can be interpreted as the characteristic time evolution of the energy observable; it gives the order of time required to see a noticeable change in the average energy of the system (and noticeable change here is equal to the energy uncertainty, ΔE). Another important conclusion here is that this time is the shortest characteristic time of the system since,

characteristic times for measurements

$$\tau_E \leq \tau_q, \qquad \tau_E = \frac{\hbar}{2\Delta E}, \qquad \tau_q = \frac{\hbar(\Delta\hat{Q})_\psi}{\left|\langle[\hat{Q},\hat{H}]\rangle_\psi\right|}$$

3.4 Examples

Time evolution of a state

Assume a quantum system in the normalized superposition state $|\psi_0\rangle$,

$$|\psi_0\rangle = \sum_{n=1}^{3} c_n|\phi_n\rangle = c_1|\phi_1\rangle + \frac{1}{2}|\phi_2\rangle + \frac{1}{2}|\phi_3\rangle, \tag{3.30}$$

expanded on the eigenbasis $|\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle$ of the energy observable, namely the system's Hamiltonian:

$$\hat{H}|\phi_n\rangle = \epsilon_n|\phi_n\rangle, \qquad n, m = 1-3 \tag{3.31}$$

$$\langle\phi_n|\phi_m\rangle = \delta_{nm}, \tag{3.32}$$

Two of the eigenvalues coincide. Let's set $\epsilon_1 = \hbar\omega_0$ and $\epsilon_2 = \epsilon_3 = 2\hbar\omega_0$.

(a) Assume that an energy measurement takes place at time $t_0 = 0$. What results one should expect and how probable they are.

(b) What is the average energy $E = \langle Q\rangle_{\psi_0}$ and the uncertainty $(\Delta H)_{\psi_0} = \Delta E_0$?

(c) Repeat the above calculations at time $t = \pi/\omega_0$

Solution. (a)

Normalization. First things first, is to normalize the state at the time of observation, which, of course is given by (3.30). The absolute value of c_1 is easily calculated by,

$$\sum_{n=1}^{3} |c_n|^2 = 1 \quad \rightarrow \quad |c_1|^2 + |\frac{1}{2}|^2 + |\frac{1}{2}|^2 = 1 \quad \rightarrow \quad c_1 = \frac{e^{\imath\theta}}{\sqrt{2}}$$

where θ is a real arbitrary number. The (relative) phase of a quantum state embedded in a linear superposition of states has a physical significance, in contrast with a phase when only one quantum state is involved (e.g. $|\psi_0\rangle$ and $e^{\imath\theta}|\psi_0\rangle$ represent the same physical state). Therefore we cannot set $\theta = 0$ or any other value. Nevertheless a good amount of information can still be extracted, even if the θ remains undetermined. So the initial state is,

$$|\psi_0\rangle = \frac{e^{\imath\theta}}{\sqrt{2}}|\phi_1\rangle + \frac{1}{2}|\phi_2\rangle + \frac{1}{2}|\phi_3\rangle. \tag{3.33}$$

Energy measurement outcomes. According to the QM postulates an *energy measurement* can provide only the eigenvalues of $\hat{H}$. In the present case only two eigenenergies will be realized, namely $\epsilon_1 = \omega_0$ and $\epsilon_2 = \epsilon_3 = 2\omega_0$ with some probability. These probabilites can be found by using the QM postulate for the expansion of a state in an eigenbasis of a physical observable, $\hat{Q}|q_n\rangle = q_n|q_n\rangle$.

Here $\hat{Q} = \hat{H}$ and $|q_n\rangle = |\phi_n\rangle$ and and $|\psi\rangle = \rangle\psi_0$. Therefore we have,

$$P(E = \epsilon_n) = |c_n|^2$$

In the present case,

$$\boxed{P(\epsilon_1 = \hbar\omega_0) = |\langle\phi_1|\psi_0\rangle|^2 = \left|\frac{e^{\imath\theta}}{\sqrt{2}}\right|^2 = \frac{1}{2}.}$$

Similarly, for the second energy eigenvalue we obtain:

$$\boxed{P(\epsilon_2 = 2\hbar\omega_0) = |c_2|^2|\langle\phi_2|\psi_0\rangle|^2 + |c_3|^2|\langle\phi_3|\psi_0\rangle|^2 = \frac{1}{4} + \frac{1}{4} = \frac{1}{2}.}$$

(b)

It is relatively trivial to calculate the expectation value of the Hamiltonian operator. One method is to use the standard definition for the average value of a quantity:

$$\langle Q\rangle = \sum_n \lambda_n P(\epsilon_n) = \hbar\omega_0 \times \frac{1}{2} + 2\hbar\omega_0 \times \frac{1}{2} = \frac{3}{2}\hbar\omega_0.$$

The above derivation was quick and straightforward. Nevertheless we also may apply the general expression for the expectation value of an operator: $\langle Q\rangle_\psi = \langle\psi|\hat{Q}|\psi\rangle$. Accordingly in the current case $\hat{Q} = \hat{H}$ and $|\psi\rangle = |\psi_0\rangle$. Then we arrive at,

$$\begin{aligned}
\langle\hat{H}\rangle_{\psi_0} = \langle\psi_0|\hat{H}|\psi_0\rangle &= \left(\frac{e^{-\imath\theta}}{\sqrt{2}}\langle\phi_1| + \frac{1}{2}\langle\phi_2| + \frac{1}{2}\langle\phi_3|\right)\hat{H}\left(\frac{e^{\imath\theta}}{\sqrt{2}}|\phi_1\rangle + \frac{1}{2}|\phi_2\rangle + \frac{1}{2}|\phi_3\rangle\right) \\
&= \left(\frac{e^{-\imath\theta}}{\sqrt{2}}\langle\phi_1| + \frac{1}{2}\langle\phi_2| + \frac{1}{2}\langle\phi_3|\right)\left(\frac{e^{\imath\theta}}{\sqrt{2}}\hat{H}|\phi_1\rangle + \frac{1}{2}\hat{H}|\phi_2\rangle + \frac{1}{2}\hat{H}|\phi_3\rangle\right) \\
&= \left(\frac{e^{-\imath\theta}}{\sqrt{2}}\langle\phi_1| + \frac{1}{2}\langle\phi_2| + \frac{1}{2}\langle\phi_3|\right)\left(\frac{e^{\imath\theta}}{\sqrt{2}}\epsilon_1|\phi_1\rangle + \frac{1}{2}\epsilon_2|\phi_2\rangle + \frac{1}{2}\epsilon_3|\phi_3\rangle\right) \\
&= \frac{1}{2}\epsilon_1 + \frac{1}{4}\epsilon_2 + \frac{1}{4}\epsilon_3 = \frac{1}{2}\hbar\omega_0 + \frac{1}{4}(2\hbar\omega_0) + \frac{1}{4}(2\hbar\omega_0) = \frac{3}{2}\hbar\omega_0,
\end{aligned}$$

where the orthonormalization condition were used for the calculation of the inner products $\langle\phi_n|\phi_m\rangle$ according the orthonormality rules of (3.32),

$$\begin{aligned}
\langle\phi_1|\phi_1\rangle = \langle\phi_2|\phi_2\rangle = \langle\phi_3|\phi_3\rangle = 1 \\
\langle\phi_1|\phi_2\rangle = \langle\phi_1|\phi_3\rangle = \langle\phi_2|\phi_3\rangle = 0.
\end{aligned}$$

An alternative method An alternative, fast track, calculation of the mean energy value can be obtained by relying in matrix operations represent operators and vectors on the (fundamental) vector basis (10)]. So, choosing $|\phi_i\rangle = |v_i\rangle = |i\rangle \;\; i = 1 - 3$, we have

$$\hat{H} = \hbar\omega_0\begin{pmatrix}1 & 0 & 0\\ 0 & 2 & 0\\ 0 & 0 & 2\end{pmatrix}, \qquad |\psi_0\rangle = \frac{1}{2}\begin{pmatrix}e^{\imath\theta}\sqrt{2}\\ 1\\ 1\end{pmatrix} \tag{3.34}$$

We then immediately get,

$$\langle \hat{H} \rangle_{\psi_0} = \langle \psi_0 | \hat{H} | \psi_0 \rangle = \underbrace{\frac{1}{2}\left(\sqrt{2}e^{-\imath\theta}, 1, 1\right)}_{\langle \psi_0 |} \cdot \underbrace{\hbar\omega_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}}_{\mathbf{H}} \cdot \underbrace{\frac{1}{2}\begin{pmatrix} \sqrt{2}e^{\imath\theta} \\ 1 \\ 1 \end{pmatrix}}_{|\psi_0\rangle} = \frac{3}{2}\hbar\omega_0$$

Uncertainty (standard deviation) The standard deviation of the system's energy at that particular time may be found by calculating ΔE using the well known statistical formula,

$$\Delta Q_\psi = \sqrt{\langle \psi | (\hat{Q} - \langle Q \rangle_\psi)^2 | \psi \rangle} = \sqrt{\langle \mathbb{Q}^2 \rangle_\psi - \langle \mathbb{Q} \rangle_\psi^2} \neq 0. \tag{3.35}$$

Replacing $\hat{Q}$ by $\hat{H}$ and using $|\psi_0\rangle$ followed by the calculation using either the abstract vector formulation in terms of bra and kets, or the matrix representation formulation on should end to $\Delta E = \hbar\omega_0/2$, shown below. It is relatively trivial to calculate the expectation value of the Hamiltonian operator (mean energy of the system) by invoking the general expression for the expectation value of an operator, $\hat{Q}$

$$\Delta H_\psi = \sqrt{\langle \psi | (\hat{H} - \langle H \rangle_\psi)^2 | \psi \rangle} = \sqrt{\langle \hat{H}^2 \rangle_\psi - \langle \hat{H} \rangle_\psi^2}. \tag{3.36}$$

Accordingly in the current case $\hat{Q} = \hat{H}$ and $|\psi\rangle = |\psi_0\rangle$. Then we arrive at,

$$\begin{aligned}
\langle \hat{H}^2 \rangle_{\psi_0} &= \langle \psi_0 | \hat{H}^2 | \psi_0 \rangle = \\
&= \left(\frac{e^{-\imath\theta}}{\sqrt{2}} \langle \phi_1 | + \frac{1}{2}\langle \phi_2 | + \frac{1}{2}\langle \phi_3 | \right) \hat{H}\hat{H} \left(\frac{e^{\imath\theta}}{\sqrt{2}} |\phi_1\rangle + \frac{1}{2}|\phi_2\rangle + \frac{1}{2}|\phi_3\rangle \right) \\
&= \left(\frac{e^{-\imath\theta}}{\sqrt{2}} \langle \phi_1 | \hat{H} + \frac{1}{2}\langle \phi_2 | \hat{H} + \frac{1}{2}\langle \phi_3 | \hat{H} \right) \left(\frac{e^{\imath\theta}}{\sqrt{2}} \hat{H}|\phi_1\rangle + \frac{1}{2}\hat{H}|\phi_2\rangle + \frac{1}{2}\hat{H}|\phi_3\rangle \right) \\
&= \left(\frac{e^{-\imath\theta}}{\sqrt{2}} \langle \phi_1 | \epsilon_1 + \frac{1}{2}\langle \phi_2 | \epsilon_2 + \frac{1}{2}\langle \phi_3 | \epsilon_3 \right) \left(\frac{e^{\imath\theta}}{\sqrt{2}} \epsilon_1 |\phi_1\rangle + \frac{1}{2}\epsilon_2|\phi_2\rangle + \frac{1}{2}\epsilon_3|\phi_3\rangle \right) \\
&= \frac{1}{2}\epsilon_1^2 + \frac{1}{4}\epsilon_2^2 + \frac{1}{4}\epsilon_3^2 = \frac{1}{2}(\hbar\omega_0)^2 + \frac{1}{4}(2\hbar\omega_0)^2 + \frac{1}{4}(2\hbar\omega_0)^2 = \frac{5}{2}(\hbar\omega_0^)2,
\end{aligned}$$

where (again) the orthonormalization condition were used for the calculation of the inner products $\langle \phi_n | \phi_m \rangle$ according the orthonormality rules of (3.32),

$$\begin{aligned}
\langle \phi_1 | \phi_1 \rangle = \langle \phi_2 | \phi_2 \rangle = \langle \phi_3 | \phi_3 \rangle = 1 \\
\langle \phi_1 | \phi_2 \rangle = \langle \phi_1 | \phi_3 \rangle = \langle \phi_2 | \phi_3 \rangle = 0.
\end{aligned}$$

An alternative method. Along similar lines as in the calculation of the mean value one may use matrix operations by representing the $\hat{H}^2$ observable in the (fundamental) vector basis (10)]. Then,

$$\hat{H}^2 = \hbar\omega_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix} \hbar\omega_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix} = (\hbar\omega_0)^2 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 4 \end{pmatrix}, \tag{3.37}$$

We then immediately get,

$$\langle \hat{H}^2 \rangle_{\psi_0} = \langle \psi_0 | \hat{H}^2 | \psi_0 \rangle = \underbrace{\frac{1}{2}\left(\sqrt{2}e^{-\imath\theta}, 1, 1\right)}_{\langle \psi_0 |} \cdot \underbrace{(\hbar\omega_0)^2 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 4 \end{pmatrix}}_{\mathbf{H}} \cdot \underbrace{\frac{1}{2}\begin{pmatrix} \sqrt{2}e^{\imath\theta} \\ 1 \\ 1 \end{pmatrix}}_{|\psi_0\rangle} = \frac{5}{2}(\hbar\omega_0)^2$$

Finally the standard deviation is

$$\Delta E_0 = \sqrt{\langle \hat{H}^2 \rangle_0 - \langle \hat{H} \rangle_0^2} = \sqrt{\frac{5}{2}(\hbar\omega_0)^2 - \frac{9}{4}(\hbar\omega_0)^2} = \frac{1}{2}\hbar\omega_0 \tag{3.38}$$

(c) Consider the time-evolved state of the latest example of measurement ($|\psi_0\rangle$).Following the general QM postulate for the time-evolution of a state, we have,

$$|\psi(t)\rangle = \sum_n c_n(0) e^{-\imath\epsilon_n t/\hbar} |\phi_n\rangle.$$

Since the $c_n(0)$ are known and $n = 1 - 3$ we end up to the following expression for the state of the current system:

$$\begin{aligned} |\psi(t)\rangle &= \frac{e^{\imath\theta}}{\sqrt{2}} e^{-\imath\epsilon_1 t/\hbar} |\phi_1\rangle + \frac{1}{2} e^{-\imath\epsilon_2 t/\hbar} |\phi_2\rangle + \frac{1}{2} e^{-\imath\epsilon_2 t/\hbar} |\phi_3\rangle \\ &= \frac{e^{\imath\theta}}{\sqrt{2}} e^{-\imath\omega_0 t} |\phi_1\rangle + \frac{1}{2} e^{-\imath 2\omega_0 t} |\phi_2\rangle + \frac{1}{2} e^{-\imath 2\omega_0 t} |\phi_3\rangle. \end{aligned}$$

At this point one repeat the calculations exactly along the lines as in the case of $|\psi_0\rangle$.

Commuting matrices and commons eigenbasis

Lets assume the fundamental basis,

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad |3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \tag{3.39}$$

the Hamiltonian of a system has matrix representation

$$\hat{H} = E_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}. \tag{3.40}$$

A second observable $\hat{Q}$ in the same fundamental basis has the matrix representation:

$$\hat{Q} = Q_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}. \tag{3.41}$$

(a) Show that indeed $|1\rangle, |2\rangle, |3\rangle$ are eigenstates of $\hat{H}$ and associate

with the corresponding eigenvalues, $E_1, E_2 = E_3$. Also show that any arbitrary combination of $|2\rangle$ and $|3\rangle$ is also an eigenvector of $\hat{H}$ with the same eigenvalue $E_2 = E_3$.

(b) Show that $[\hat{Q}, \hat{H}] = 0$.

(c) Solve the eigenvalue equation for $\hat{Q}$ and find its eigenvalues and eigenvectors.

(d) If the eigenvectors of $\hat{Q}$ are named $|q_1\rangle, |q_2\rangle, |q_3\rangle$ then show that these eigenvectors are also eigenvectors of $\hat{H}$.

(e) Rename $|q_1\rangle, |q_2\rangle, |q_3\rangle$ so that to include information about both the $\hat{H}$ and $\hat{Q}$ eigenvalues.

(f) A measurement of the energy and the $\hat{Q}$ gave as a result the values $2E_0$ and $-Q_0$ respectively. What is the state of the system after the measurements?

Solution: (a)

It is straightforward to show by explicitly invoking the matrix representation of $\hat{H}$ and the column-representation of $|1\rangle, |2\rangle, |3\rangle$ that:

$$\begin{aligned} \hat{H}|1\rangle &= E_0|1\rangle, \qquad E_1 = E_0 \\ \hat{H}|2\rangle &= 2E_0|2\rangle, \qquad E_2 = E_0 \\ \hat{H}|3\rangle &= 2E_0|3\rangle, \qquad E_3 = E_0, \end{aligned}$$

This way have associated the possible eigenvalues with the eigenstates $|1\rangle, |2\rangle, |3\rangle$. However we see that this Hamiltonian has E_2 equal to E_3, namely, $E_2 = E_3 = 2E_0$. This means that if we measure the energy of the system and obtained $2E_0$ then we would no have any clue as to which of the states $|2\rangle$ or $|3\rangle$ the system resulted. How then we can distinguish between $|2\rangle$ and $|3\rangle$? To our resque the solution is to perform some other measurement of some suitable observable; this will help us to distinguish among the two possible states, resulting from the energy measurement. The 'suitable' observable here is an observable which commutes with the Hamiltonian.

Next, let's choose an arbitrary vector in the space spanned by the degenerate eigenstates:

$$|e\rangle = a|2\rangle + b|3\rangle. \tag{3.42}$$

We'll know check whether this is an eigenvector of $\hat{H}$. For this, the following should hold:

$$\hat{H}|e\rangle = E_2|e\rangle, \quad \text{or } E_3 \text{ since } E_2 = E_3.$$

Then we have,

$$\begin{aligned} \hat{H}|e\rangle &= \hat{H}(a|2\rangle + b|3\rangle) = a\hat{H}|2\rangle + b\hat{H}|3\rangle \\ &= aE_2|2\rangle + bE_3|3\rangle = E_2(a|2\rangle + b|3\rangle) = E_2|e\rangle, \end{aligned}$$

since $\hat{H}|2\rangle = E_2|2\rangle$ and $\hat{H}|3\rangle = E_3|3\rangle$ and $E_2 = E_3 = 2E_0$.

This property of degenerate eigenstates is general and gives the freedom to choose any set of orthonormal set of eigenstates in the 'plane' of $|2\rangle, |3\rangle$ as expressed in (3.42). This extra degree 'freedom' property will be used below to uniquely characterize the state of the system, by finding suitable a, b that makes the states $|e\rangle$ eigenstates not only of the Hamiltonian but also of another suitable observable.

(b)

To prove that $[\hat{Q}, \hat{H}] = 0$ is equivalent to show that $\hat{H}\hat{Q} = \hat{Q}\hat{H}$. In matrix representation one has to confirm that: [52]

$$E_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix} \cdot Q_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} = Q_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \cdot E_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}$$

The vanishing commutator means that there is a set of eigenvectors which are common to the $\hat{H}$ and the $\hat{Q}$ observables. [53]

(c)

Since a matrix representation of the operator is available a standard matrix diagonalization suffices to find the observable's eigenvalues.

$$\hat{Q}|q\rangle = \lambda|q\rangle \rightarrow \quad \begin{pmatrix} Q_0 & 0 & 0 \\ 0 & 0 & Q_0 \\ 0 & Q_0 & 0 \end{pmatrix} \cdot \begin{pmatrix} C_1 \\ C_2 \\ C_3 \end{pmatrix} = \begin{pmatrix} \lambda & 0 & 0 \\ 0 & \lambda & 0 \\ 0 & 0 & \lambda \end{pmatrix} \cdot \begin{pmatrix} C_1 \\ C_2 \\ C_3 \end{pmatrix}$$

where we want to find the orthonormalized eigenvectors,

$$\lambda \quad \text{and} \quad |q\rangle = \begin{pmatrix} C_1 \\ C_2 \\ C_3 \end{pmatrix}.$$

Moving everything from one side of the equation.

$$(\mathbf{Q} - \lambda \mathbb{1})\,|q_n\rangle = 0, \qquad \rightarrow \quad \begin{pmatrix} Q_0 - \lambda & 0 & 0 \\ 0 & -\lambda & Q_0 \\ 0 & Q_0 & -\lambda \end{pmatrix} \cdot \begin{pmatrix} C_1 \\ C_2 \\ C_3 \end{pmatrix} = 0$$

The possible eigenvalues can be simply found as the roots of the determinant of $((\mathbf{Q} - \lambda \mathbb{1})$ matrix:

$$\begin{aligned} det\,(\mathbf{Q} - \lambda \mathbb{1}) = 0 \quad &\rightarrow \quad (Q_0 - \lambda)(Q_0^2 - \lambda^2) = 0 \\ &\rightarrow \quad (Q_0 - \lambda)^2(Q_0 + \lambda) = 0 \quad \rightarrow \quad \lambda = \pm Q_0. \end{aligned}$$

We then have two eigenvalues one appearing once $\lambda = -Q_0$ and the other $\lambda = +Q_0$ (we say then that it is *doubly degenerate*).

At this point it is left as an exercise to the reader to calculate the normalized eigenvectors, $|q_1\rangle, |q_2\rangle, |q_3\rangle$. The results are as below

$$|q_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \qquad |q_2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}, \qquad |q_3\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix}, \tag{3.43}$$

52: I assume here that the reader will check this.

53: Here you can convince yourself that none of the $|1\rangle, |2\rangle, |3\rangle$ are eigenvectors of $\hat{Q}$. How can you do that? For example you can show that,

$$\hat{Q}|1\rangle \neq c\,|1\rangle.$$

for any real number, c.

It is trivially seen that it is an orthonormalized basis since $\langle q_i|q_j\rangle = \delta_{ij}$ for any combination of $i, j = 1-3$ [54].

54: The reader should also check this.

(d) Again now it is straigforward to convince ourselves that these eigenstates are also eigenstates of the Hamiltonian observable by ensuring that for the three energy eigenvalues holds:

$$\begin{aligned}\hat{H}|q_1\rangle &= E_0|q_1\rangle,\\ \hat{H}|q_2\rangle &= 2E_0|q_1\rangle,\\ \hat{H}|q_3\rangle &= 2E_0|q_1\rangle,\end{aligned}$$

So we have $E_1 = E_0$, $E_2 = 2E_0$ and $E_3 = 2E_0$ associated with the $|q_1\rangle, |q_2\rangle, |q_3\rangle$ eigenvectors, respectively.

(d)

From the results of question (c) we can rename the common eigenvectors so that in their definition to be characterized by the eigenvalues of both $\hat{H}$ and $\hat{Q}$ observables. The results maybe summarized in the following table:

n	q_n	E_n	$\lvert E_n, q_n\rangle$
1	Q_0	E_0	$\begin{pmatrix}1\\0\\0\end{pmatrix}$
2	Q_0	$2E_0$	$\frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\1\end{pmatrix}$
3	$-Q_0$	$2E_0$	$\frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\-1\end{pmatrix}$

In particular the corresponding eigenvalue equations are as below:

$$\begin{aligned}\hat{H}|E_n, q_n\rangle &= E_n|E_n, q_n\rangle\\ \hat{A}|E_n, q_n\rangle &= q_n|E_n, q_n\rangle.\end{aligned}$$

(f)

In QM terminology such a set of observables with common eigenstates is known as *complete set of commuting observables (CSCO)*. This set is *complete* because the measurement of $\hat{H}$ and $\hat{Q}$ is sufficiently to specify uniquely the state of the system, given the outcome of the measurements. So for the given set of measurements we immediately conclude that the system resulted to the eigenstate $|E_3, q_3\rangle$

Measurements on a specific state

The system of the previous example is in the state

$$|\psi\rangle = \frac{1}{\sqrt{3}}|1\rangle + \sqrt{\frac{2}{3}}|2\rangle \tag{3.44}$$

(a) What is the probability of measuring energy E_0 or $2E_0$?

(b) What is the probability of measuring energy E_0 and $-Q_0$

Solution First thing is to check whether the state is normalized. One can immediately see that indeed

$$|\frac{1}{\sqrt{3}}|^2 + |\sqrt{\frac{2}{3}}|^2 = \frac{1}{3} + \frac{2}{3} = 1$$

add up to unity

(**a)** To answer this question the given expression for $|\psi\rangle$ is sufficiently informative and we can immediately recall the QM principles to conclude that the corresponding probabilities for the energy measurements are:

$$P_\psi(E = E_0) = |\frac{1}{\sqrt{3}}|^2 = \frac{1}{3}, \qquad P_\psi(E = 2E_0) = |\sqrt{\frac{2}{3}}|^2 = \frac{2}{3}$$

(b) For the second set of measurements an extra measurement was performed for the $\hat{Q}$ observable. In this case we need to express the state $|\psi\rangle$ in terms of the common eigenstates of $\hat{H}$ and $\hat{H}$, namely the $|E_n, q_n\rangle, n = 1, 2, 3$ basis. Straightforward manipulations result to the following relations between $|1\rangle, |2\rangle, |3\rangle$ and $|E_n, q_n\rangle, n = 1, 2, 3$ bases: [55]

55: essentially this is the equivalent of change of a coordinate system in the 3-D physical vector space

$$|E_0, Q_0\rangle = |1\rangle$$
$$|2E_0, Q_0\rangle = \frac{1}{\sqrt{2}}(|2\rangle + |3\rangle) \qquad |2E_0, -Q_0\rangle = \frac{1}{\sqrt{2}}(|2\rangle - |3\rangle)$$

Therefore reversing the relations we have,

$$|1\rangle = |E_0, Q_0\rangle \quad |2\rangle = \frac{1}{\sqrt{2}}(|2E_0, Q_0\rangle + |2E_0, -Q_0\rangle)$$

Now we substitute the above expressions in the $|\psi\rangle$ state (3.44) to obtain,

$$|\psi\rangle = \frac{1}{\sqrt{3}}(|E_0, Q_0\rangle + |2E_0, Q_0\rangle + |2E_0, -Q_0\rangle). \tag{3.45}$$

From the above expression we can now obtain immediately the probability obtaining the the values $2E_0$ and $-Q_0$ upon measurements of $\hat{H}$ and $\hat{Q}$:

$$P(E = 2E_0, Q = -Q_0) = |\frac{1}{\sqrt{3}}|^2 = \frac{1}{3}.$$

Note that the resulting expression is also normalized, as it should be, of course.

Question 3.4.1

What is the commutator $[\hat{S}_z, \hat{S}_x]$ if

$$\hat{S}_z = \frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}, \qquad \hat{S}_x = \frac{\hbar}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$$

Solution The commutator then becomes a matrix multiplication:

$$\hat{S}_z\hat{S}_x = \frac{\hbar^2}{4}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} = \frac{\hbar^2}{4}\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix} \tag{3.46}$$

and

$$\hat{S}_x\hat{S}_z = \frac{\hbar^2}{4}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} = \frac{\hbar^2}{4}\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}. \tag{3.47}$$

Subtracting these, we get

$$[\hat{S}_z, \hat{S}_x] = \frac{\hbar^2}{2}\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix} = \imath\hbar\hat{S}_y. \tag{3.48}$$

It looks like the commutator has a circular relationship.

The commutator has units $\hbar^2$ since we are multipling two spins. The result $\imath\hbar\hat{S}_y$ has the same units, so we are good.

3.5 Questions

Question 3.5.1

Assume a quantum system with a Hamiltonian $\hat{H}$ and an observable operator $\hat{A}$ given, represented in the same (fundamental) basis by,:

$$\hat{H} = \begin{pmatrix} E_0 & 0 & 0 \\ 0 & 2E_0 & 0 \\ 0 & 0 & 3E_0 \end{pmatrix} \qquad \hat{A} = \begin{pmatrix} A_0 & 0 & 0 \\ 0 & 2A_0 & 0 \\ 0 & 0 & A_0 \end{pmatrix}. \tag{3.49}$$

The state of the system at time $t_0 = 0$;

$$|\psi(0)\rangle = \frac{1}{3}\begin{pmatrix} 1 \\ \imath \\ \sqrt{7} \end{pmatrix} \tag{3.50}$$

(a) What is $|\Psi(t)\rangle$ for $t > 0$?
(b) If $\hat{H}$ is measured at $t > 0$, what are the possible energy results and what are the corresponding probabilities? What is the state of the system after each of the possible measurements?
(c) If, instead, $\hat{A}$ is measured at $t > 0$, what are then the possible results? What are the respective probabilities?
(d) Calculate $\langle \hat{A} \rangle_\psi$ and the uncertainty $(\Delta \hat{A})_\psi$

Question 3.5.2

Consider a system characterized by a Hamiltonian $\hat{H}$ and observable $\hat{Q}$ that is in the state

$$|\psi(t=0)\rangle = \frac{1}{2}|1\rangle + \frac{\imath}{2}|2\rangle - \frac{1}{\sqrt{2}}|3\rangle \tag{3.51}$$

(a) Find $|\psi(t > 0)\rangle$.
(b) If we measure $\hat{Q}$ at $t > 0$, find the average of the results.
(c) What is the uncertainty in the measurement of $\hat{Q}$?

3.6 Some conclusive comments

Having investigated even deeper the consequences derived from the QM principles in simple quantum systems, without having actually put these systems in any physical context; that is we talked about Hamiltonian, spins and 'observables' without further specifying the physical system under consideration; for example the Hamiltonian might refer to the energy observable of the hydrogen atom or a free electron. The spin we have discussed could equally refer to the electron's intrinsic spin state or to the Calcium's nuclei spin, and so on.

It is now the time that we become more specific; we are armed though with some basic tools and concepts, namely the QM principles and a mathematical formulation. We are ready to discuss more closely these dynamical quantities (observables in QM) which are used (upon their measurement operations) to characterize a quantum system. Some of these observables are as useful as in Classical Mechanics, i.e. the position and momentum (linear), the energy, angular momentum etc. However other have no classical counterpart with the chief example the spin observable. It is a purely *quantum* observable.

In the next chapters we'll go through these, more specific, investigations and will apply the QM principles accordingly, adapted/amended or augmented. For example by 'adapted' here we can think the case of the position; this observable, upon measurement, may give as a result any position in space (in general) which means that the measurements are of *continuous* nature rather than of *discrete* as we have assumed to date for simplicitly reasons. Thus we need to adapt the QM expressions accordingly; needless to say that this is possible, nevertheless not that it was a mathematically trivial case.

In addition we'll also investigate the motion of a quantum particle (i.e. electron) under a free-field environment (free-particle, $V(x) = 0$) or under an harmonic potential field, $V(x) = kx^2/2$. The former case describes an electron of unbound motion possesing only kinetic energy, $E = p^2/2m$ while in the latter case of harmonic potential we'll see that the electron (or any other particle) possess discrete energies, nevertheless its motion is generally restricted. [56]. The hydrogen atom can be treated under the assumption that the electron moves in the proton's Coulomb field with potential energy $V(r) = -Kq/r$; it results that its energy can be discrete or continuous while its motion range can be bounded or infinite (ionized hydrogen).

56: A system which is often described with such potential is the so-called, *quantum dot* (or artificial atom). Quantum dots share many properties similar to the physical atomic systems, such as the electronic structure.

Wave Mechanics: QM in position basis

4

4.1 Wavefunctions as components of the position basis

According to QM a set of basis states $|q\rangle$, being eigenvectors of an observable, $\hat{Q}$, can decompose any arbitrary quantum state:

$$|\psi\rangle = \sum_q c_q |q\rangle, \qquad c_q = \langle q|\psi\rangle, \tag{4.1}$$

where c_q where interpreted as the components of ψ in the basis $|q\rangle$. It's physical interpretation is that:

$$\text{Prob}\{\hat{Q} = q\} = |c_q|^2 = |\langle q|\psi\rangle|^2.$$

Nevertheless, this formulation includes only those physical observable which take discrete values with notable example the spin observable of a particle.

[58] While spin is an observable which takes exclusively discrete values this is not the case for other observables such the energy and the momentum for example. Energy for example may take discrete values but it can also be the case that takes continuous values; the former case includes all bound systems while the latter all unbound ones (e.g. free particles). Furthermore the position of a particle is assumed that it takes only continuous values. Since very often it makes sense to ask the position of a particle it is natural to design a position measurement and to associate an QM observable; namely the position observable. Thus, the position observable is a characteristic example of a continuous QM observable.

58: Here the term 'particle' is used to include a variety of quantum entities, e.g. elementary or compound particles such as electrons, protons, atoms, molecules, etc..

Therefore we need to include the possibility of *continuous* spectrum of an observable [59]. Since the eigenvectors are continuous, we need to describe the components α_λ in terms of a continuous function instead of discrete complex values. We define this new parameter as $\psi(\lambda)$, a complex-valued function of λ.

59: The use of 'spectrum' in this context means that an observable may acquire continuous set of eigenstates and of course each of these is accompanied by a eigenvalue. Accordingly, an observable with discrete spectrum has discrete set of eigenstates/eigenvalues. Note that a system may have discrete and continuous spectrum. For example energy or momentum.

We talked about the position observable but the generalization should include any continuous observable. Thus representing such an observable, say by $\hat{\Lambda}$, let's assume that the eigenvalue problem has been solved and its eigenbasis has determined:

$$\hat{\Lambda}|\lambda\rangle = \lambda|\lambda\rangle, \qquad \sum_\lambda |\lambda\rangle\langle\lambda| = \mathbb{1}, \qquad \langle\lambda|\lambda'\rangle = \delta_{\lambda\lambda'}$$

Then, it can be shown that the arbitrary quantum state may be decomposed formally in the continuous basis,

$$\begin{aligned}
|\psi\rangle = \sum_\lambda \psi_\lambda |\lambda\rangle \qquad &\rightarrow \qquad |\psi\rangle = \int_\lambda d\lambda \psi(\lambda)|\lambda\rangle \\
\mathbb{1} = \sum_\lambda |\lambda\rangle\langle\lambda| \qquad &\rightarrow \qquad \int d\lambda |\lambda\rangle\langle\lambda| = \mathbb{1}. \\
\delta_{\lambda\lambda'} = \langle\lambda|\lambda'\rangle \qquad &\rightarrow \qquad \delta(\lambda - \lambda') = \langle\lambda|\lambda'\rangle
\end{aligned}$$

In words, the sums, $\sum_\lambda$, become integrals and the discrete components, psi_λ become continuous functions and the Kronecker symbol, $\delta_{\lambda,\lambda'}$, generalizes to the so-called Dirac-delta function. In this context the continuous-valued components, $\psi(\lambda)$,

$$\psi(\lambda) = \langle \lambda | \Psi \rangle \,. \tag{4.2}$$

are called *wavefunctions* and essentially describe completely the quantum state $|\Psi\rangle$ in the λ basis [60] .

60: When the continuous-valued observable happens to be the position observable, $\hat{\Lambda} = \hat{x}$, the continuous component $\psi(\lambda)$ is nothing else than the familiar spatial wavefunction, $\psi(x)$:

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

Continuous Probability distribution

$$\text{Prob}_\psi\{ \text{ Measurement of } \hat{\Lambda} \quad \text{in} \quad [\lambda, \lambda + d\lambda] \} = dP_\psi(\lambda) = dx|\psi(\lambda)|^2,$$

Therefore, $|\psi(\lambda)|^2$ is the $\hat{\Lambda}$-observable's measurement outcomes *probability distribution*. If $\hat{\Lambda}$ is known to take values between a, b then, in line to this statistical intrepretation we should have [61] ,

$$\int_a^b dP_\psi(\lambda) = \int_a^b d\lambda |\psi(\lambda)|^2 = 1. \tag{4.3}$$

61: Of course a, b may take infinite values e.g. $[a, b] = [-\infty, \infty]$ or $[a, b] = [0, \infty]$. This depends on the observable under consideration. In passing, in order to simplify notation we make the following assumption:

$$\int_{-\infty}^{+\infty} \to \int$$

So, if in the integration symbol if the limits are not explicitly shown, then it should be taken as granted that cover the full range of the real axis.

It is important to bear in mind the following general rule of QM:

Square integrable wavefunctions

A quantum state can only be associated to a physical state if it can be represented by a wavefunction which is *square integrable*, namely the integral of its absolute square to be finite, that is:

$$\int_a^b d\lambda |\psi(\lambda)|^2 = C < \infty$$

The last important add in the towards the generalization to the continuum QM states is the definition of the inner product in such quantum vector states (of infinite dimension, complex and continuous valued vectors). So for two arbitrary QM vectors, ψ and ϕ expanded on the eigenbasis of a continuously-valued observable their inner-product is defined to be [62] ,

62: A detailed proof of this expression will be given in the later section in the context of the position observable.

Inner product in continuous-valued QM vector space

$$\langle \psi | \phi \rangle = \int d\lambda \, \psi^*(\lambda) \phi(\lambda) \tag{4.4}$$

In order to be more specific in the below we'll examine the case of the two most important observables in both classical and quantum mechanics, namely the position and momentum observables. They owe their importance on the actual fact that most of the physical quantities concerning the motion of a system in space are expressed in terms of these quantities; e.g. angular momentum, $\mathbf{L} = \mathbf{r} \times \mathbf{p}$, energy, $E = p^2/2m + V(x)$.

4.2 Position Basis

[63] The goal here is to establish the QM rules which model the behavior of a single particle confined to move in a single dimension. We wish to work in the position basis, $|x\rangle$, which describes the quantum position eigenvectors of the particle. According to QM the arbitrary vector state ψ maybe expanded in the position basis by using the linear superposition principle, with a careful generalization of the discrete sums and the Kronecker-symbol to its continued-valued mathematical objects, [64]:

$$\sum_i \quad \rightarrow \quad \int dx, \qquad \delta_{ij} \rightarrow \delta(x_i - x_j) \tag{4.7}$$

In this case we have,

Position superposition principle and wavefunction

$$|\psi\rangle = \int_{-\infty}^{+\infty} dx \psi(x)|x\rangle, \qquad \langle\psi| = \int_{-\infty}^{+\infty} dx \psi^*(x)\langle x| \tag{4.8}$$

property.

In this basis, the quantity which links a possible QM particle state, ψ, with the outcomes of a position measurement is the spatial wavefunction, given by,

$$\psi(x) = \langle x|\psi\rangle \quad \text{and} \quad \psi^*(x) = \langle\psi|x\rangle\,. \tag{4.9}$$

All the information about the QM state ψ now is contained in the $\psi(x)$. Therefore we must be in a position to 'extract' information about quantities of interest, such as QM averages of various operators, outcomes of measurements together with the time-evolution of the particle's state; that is possible provides, $\psi(x)$ is known.

Before doing this we should consider the corresponding generalization of the eigenvalue equation for the position operator:

Position operator and eigenbasis

The eigenvalue equation for the position observable is:

$$\hat{X}|x'\rangle = x'|x'\rangle, \qquad \int dx|x\rangle\langle x| = \mathbb{1}, \qquad \langle x|x'\rangle = \delta(x - x')$$

Now following the rule about the wavefunction (as component), $\psi(x)$ of the quantum vector state ψ we see that the corresponding wavefunction of the eigenstate vector $|x'\rangle$ we have,

$$\psi_{x'}(x) = \langle x|x'\rangle = \delta(x - x') = \begin{cases} \infty, & x = x' \\ 0 & x \neq x' \end{cases}, \tag{4.10}$$

63: **The Dirac-delta function**: It may be defined by the following property:

$$\delta(x - x') = \begin{cases} \infty, & x = x' \\ 0 & x \neq x' \end{cases}$$

or it may be defined by its following property,

$$\int_{-\infty}^{+\infty} \delta(x - x')f(x')dx' = f(x) \tag{4.5}$$

In effect, it is zero everywhere except at one point x where it is, in effect, infinite. The function $F(x')$ could be a constant in which case

$$\int_{-\infty}^{+\infty} \delta(x - x')dx' = 1. \tag{4.6}$$

64: In the class lectures it was described in detail how this is done

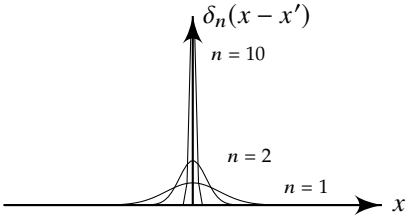


Figure 4.1: The Dirac-delta function maybe approximated with a variety of conventional function via a limiting procedure. For example via a Gaussian function $n \rightarrow \infty$:

$$\delta_n(x) = \frac{n}{\sqrt{\pi}} e^{-(n(x-x'))^2} \rightarrow \delta(x - x')$$

Thus, the eigenfunctions of the position operator is a rather peculiar mathematical object, where is everywhere zero and only at one point takes the value of infinite, namely at the eigenvalue point, x'. So if we strictly follow the statistical interpretation about the wavefunctions of a system then we conclude that,

$$\text{Prob}_{\psi_{x'}}\{\hat{X} \;\; in \;\; [x', x'+dx]\} = dP_{\psi_{x'}}(x') = dx|\psi'_x(x)|^2 = dx\delta^2(x-x') = \infty,$$

But, by the very rules of probability theory, no probability can have value larger than one. We then arrive at the conclusion that the eigenfunctions of the position operator are not associated with any physically realistic state of a system [65] .

65: Strictly speaking, it is the integral, $\int dP_{\psi_{x'}}(x') = \int dx\delta^2(x-x') = \infty$ that should be finite. But it is not, due to the presence of the square of the Dirac-delta function.

Improper and proper wavefunctions

The system's eigenstates $|x\rangle$ associated with wavefunctions $\psi_{x'}(x) = \delta(x-x')$ that do not have finite normalization and as such they cannot be realized; in other words they do not describe any physical state; we may say that they are improper QM states. Nevertheless, suitable linear combination of these improper states (superposition principle) may lead to proper states.

Inner products in position basis

Let's now use the above to obtain the inner product between two quantum states in the position basis: Take two arbitrary states, ψ and ϕ expressed in the position basis:

$$|\psi\rangle = \int dx\psi(x)|x\rangle, \qquad |\phi\rangle = \int dx\phi(x)|x\rangle,$$

then [66] ,

66: The proof to this goes as follows:

$$\begin{aligned}\langle\psi|\phi\rangle &= \int dx\psi^*(x)\langle x| \int dx'\phi(x')|x'\rangle \\ &= \int\int dxdx' \langle\psi|x\rangle \langle x|x'\rangle \langle x'|\phi\rangle \\ &= \int\int dxdx'\psi^*(x)\delta(x-x')\phi(x') \\ &= \int dx\psi^*(x)\phi(x)\end{aligned}$$

where we used the definition of the wavefunction, Eq. (4.2), to write the inner product in terms of the wavefunctions in the position basis. Since our quantum states are normalized, the inner product of a quantum state with itself is one:

Inner product in the position basis

$$\langle\psi|\phi\rangle = \int dx\psi^*(x)\phi(x) \tag{4.11}$$

The above definition ensures that an arbitrary state $|\psi\rangle$ expressed in the position basis is automatically normalized since, for $|\phi\rangle = |\psi\rangle$ we have,

$$\langle\psi|\psi\rangle = \int dx\psi^*(x)\psi(x) = \int dx|\psi(x)|^2 = 1. \tag{4.12}$$

which is nothing else than the normalization condition [67] .

67: From the normalization condition it is easily concluded that the wavefunction in the position basis also has units $[\text{m}^{-1/2}]$

Measurement and averages

First we need to clarify once for ever the connection between $\psi(x)$ and outcomes of position measurements. This, in accordance with the standard interpretation of the c_n amplitudes when a state expanded

in terms of the eigenbasis of a discrete observable, since now the $\psi(x)$ play the same role for the position operator, naturally the below holds:

Probability distribution of position measurements

$$\text{Prob}_\psi\{\text{Measurement of } \hat{x} \;\; in \;\; [x, x+dx]\} = dP_\psi(x) = dx|\psi(x)|^2,$$

Therefore, $|\psi(x)|^2$ is actually a spatial *probability density distribution*[68] for finding the particle somewhere in space. In accordance to the requirement that the particle should be found somewhere with certainty it is concluded that the integration over the whole space, should give,

$$\int dP(x) = \int_{-\infty}^{+\infty} dx|\psi(x)|^2 = 1.$$

Accordingly, given that the system/particle is in a state $\psi(x)$ we can calculate the probability that a position measurement will find the particle between the position points a and b:

$$P_\psi(a,b) = \int_a^b dx|\psi(x)|^2. \tag{4.13}$$

68: Maybe it is useful to assign a special symbol to it, $\mathcal{P}(x) = |\psi(x)|^2$ and therefore,

$$\mathcal{P}(x) = \frac{dP(x)}{dx} \quad \leftrightarrow \quad P(x) = \int_a^x dx' \mathcal{P}(x')$$

In this case we may call $P(x)$ as *probability distribution* (The dependence in ψ has been dropped for convenience; otherwise, more accurately we should have write, P_ψ and $\mathcal{P}_\psi$. With these definition, $P(a) = 0$ and $P(\infty) = 1$.

4.3 Momentum observable in the position basis

One can start with eigenvalue equation of the momentum operator; namely by investigating the action of the momentum operator on a momentum eigenstate. Let's denote the momentum operator (in 1-D) as, $\hat{P}_x$ and the associated eigenstates as $|p_x\rangle$; so $|p_x\rangle$ describes a particle with definite momentum p_x. However there is a basic difference between the position and the momentum observable which will show up later: a particle may be in a state where its momentum may take values that are discretized or continuous or both. For now, we'll be using the notation $|p_x\rangle$ to include both cases. The eigenvalue equation for the momentum is:

$$\hat{P}_x|p_x\rangle = p_x|p_x\rangle \tag{4.14}$$

How we solve this equation and determine the corresponding eigenfunctions? To this end we multiply from the left by $\langle x|$ and consider the general rule where the wavefunctions of a state $|\psi\rangle$ in the position basis are expressed as, $\psi(x) = \langle x|\psi\rangle$. In addition we need to supplement this rule by the following general rules[69]

69: Lets take these unproved for now.

position and momentum operators action on a state $|\psi\rangle$

$$\langle x|\hat{P}_x|\psi\rangle \equiv \hat{p}_x\psi(x) = -\imath\hbar\frac{\partial}{\partial x}\psi(x), \qquad \langle x|\hat{X}|\psi\rangle \equiv x\psi(x) \tag{4.15}$$

A short-hand rule for the expression of the momentum and position operator in the position basis is,

position and momentum operators

$$\hat{X} \quad \rightarrow \quad \hat{x} = x, \qquad \hat{P}_x \quad \rightarrow \quad \hat{p}_x = -\imath\hbar\frac{\partial}{\partial x} \tag{4.16}$$

So here we have,[70]

$$\hat{P}_x|p_x\rangle = p_x|p_x\rangle \quad \rightarrow \quad \langle x|\hat{P}_x|p_x\rangle = p_x\,\langle x|p_x\rangle$$
$$-\imath\hbar\frac{d}{dx}\psi_p(x) = p_x\psi_p \quad \rightarrow \quad \psi_p(x) = Ne^{\imath\frac{p_x}{\hbar}x}$$

70: Clarification about the symbols may be required at this point. First, $\psi_p(x) = \langle x|p_x\rangle$ is the eigenfuction of the momentum observable in the position basis. $\hat{P}_x$ is the symbol for the momentum observable generally (not tied to any eigenbasis). $\hat{p}_x = -\imath\hbar\frac{\partial}{\partial x}$ is the symbol for the momentum observable expressed in the position basis $|x\rangle$. Finally, p_x is the eigenvalue of the momentum eigenstate $|p_x\rangle$.

So we arrive at the momentum eigenfunction in the position basis to be of the following form:

$$\psi_p(x) = \langle x|p_x\rangle = Ne^{\imath\frac{p_x}{\hbar}x}. \tag{4.17}$$

The N is a constant the value of which will be determined by the normalization condition requirement, if we want to interpret $|\psi_p(x)|^2$ as probability distributions. During the normalization procedure it turns out that we need to consider two different cases (a) when the particle is

bound to move in a restricted space (e.g. electrons in atoms/molecules/nano-sized materials) and (b) the particle is free to move without boundaries or at least can be considered infinitely large for all practical purposes (e.g. electron/molecule gases, particles in accelerator beams etc..). So let's start with the bounded case:

Bounded particles. We need to set up a coordinate system to count the particle's position, x. Since the 1-D region is finite (say of length L) we can choose its origin to be at the of the region or at its middle point; obviously, either choice should lead to the same physical predictions. For convenience we choose the origin at the middle of the interval. We also take as granted that the available region is free from any potential field and as such for symmetry reasons we should assume the same values for the particle's wavefunction at the two boundary points, that is:

$$\psi_p(x = -\frac{L}{2}) = \psi_p(x = +\frac{L}{2}). \tag{4.18}$$

This choice of the boundary conditions (BC) ensures that the particle has the same probability to be found at the two sides of the region (since $|\psi(-L/2)|^2 = |\psi(L/2)|^2$) [71] . First we apply the normalization condition in order to determine the normalization constant, N:

$$1 = \langle p|p\rangle = \int_{-\frac{L}{2}}^{+\frac{L}{2}} dx|\psi_p(x)|^2 = \int_{-\frac{L}{2}}^{+\frac{L}{2}} |Ne^{\imath\frac{p_x}{\hbar}x}|^2 = |N|^2 \int_{-\frac{L}{2}}^{+\frac{L}{2}} dx = |N|^2 L.$$

71: In fact any boundary conditions of the form

$$\psi_p(-\frac{L}{2}) = e^{\imath\phi}\psi_p(\frac{L}{2})$$

with ϕ arbitrary are also possible.

Thus we arrive at the following value:

$$N_\theta = e^{\imath\theta}\sqrt{\frac{1}{L}} \qquad \rightarrow \qquad N = \frac{1}{\sqrt{L}},$$

where we set $\theta = 0$ as there is no any physical significance in the values of θ.

Applying these BC conditions in (4.17) we find,

$$e^{\imath\frac{p_x L}{2\hbar}} = e^{-\imath\frac{p_x L}{2\hbar}} \rightarrow e^{\imath\frac{2p_x L}{2\hbar}} = 1 \rightarrow \cos\frac{p_x L}{\hbar} + \imath\sin\frac{p_x L}{\hbar} = 1$$

The above relation leads to,

$$\frac{p_x L}{\hbar} = n\pi \qquad \rightarrow \qquad p_n = \hbar\frac{n\pi}{L}, \quad n = 0, \pm1, \pm2, \cdots$$

Here the notation was changed from $p_x \rightarrow p_n$ to emphasize that if the particle is bound in a region of space say L the momentum eigenvalues, p_x are discretized. By recalling the relation between momentum and wavenumber, $p_x = \hbar k_x$ and the relation of the wavelengths with the wavenumber, $\lambda = 2\pi/k_x$ then we see that these quantities are also discretized:

$$k_n = \frac{n\pi}{L}, \qquad \lambda_n = \frac{2L}{n}, \qquad n = 0, \pm1, \pm2, \cdots \tag{4.19}$$

Finally we can summarize:

Bounded particles in momentum state $|p_n\rangle$

The momentum eigenfunctions are normalizable and represent a particle in a physical state of momentum p_n:

$$\psi_{p_n}(x) = \langle x|p_n\rangle = \frac{1}{\sqrt{L}} e^{\imath \frac{p_n x}{\hbar}}, \qquad -\frac{L}{2} \leq x \leq \frac{L}{2} \tag{4.20}$$

$$\langle p_n|p_m\rangle = \delta_{nm}, \qquad p_n = \frac{n\pi}{L}, \quad n = 0, \pm 1, \pm 2, \cdots$$

$|\psi_{p_n}(x)|^2$, Prob{ a position measurement in (x,x+dx)}.

Since we have determined the eigenfunctions of the momentum observable for a bounded particle((which now we associate with a discrete vector state $|p_n\rangle$) then according to QM postulates any physical state of the particle can be expanded on these momentum eigenstates.

Expansion on momentum states (bounded particle)

$$|\psi\rangle = \sum_n c_{p_n} |p_n\rangle, \qquad \rightarrow \qquad \psi(x) = \sum_n c_{p_n} \phi_n(x) \tag{4.21}$$

$|c_{p_n}|^2$, Prob{ a momentum measurement will give p_n}. (4.22)

We then see that the quantity $|c_{p_n}|^2$ gives the probability that a momentum measurement will provide the associated eigenvalue p_n.

Unbounded particles, $L \rightarrow \infty$.

The situation is different for unbounded particles that can move freely anywhere in space. It was shown in the lectures that these states are unnormalized and therefore cannot represent physical states. Nevertheless suitable linear combinations of them can be used to represent realistic physical states. At this point we refrain to elaborating more on the mathematical details of the derivation which was presented in the lectures [72] and only present the final formulas for the momentum eigenstates of unbounded particles:

Unbounded particles

$$\psi_{p_x}(x) = \langle x|p_x\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{\imath \frac{p_x x}{\hbar}}, \qquad -\infty \leq x \leq \infty \tag{4.23}$$

$$\langle \psi_{p_x}|\psi_{p'_x}\rangle = \delta(p_x - p'_x) = \begin{cases} \infty, & p_x = p'_x \\ 0, & p_x \neq p'_x. \end{cases}$$

$|\psi_p(x)|^2$, Prob{ a position measurement in (x,x+dx)}.

Again, having solved the eigenvalues and produced the momentum eigenbasis an arbitrary quantum state maybe now expressed in terms of this eigenbasis. In an abstract notation one has:

72: Nevertheless, an alternative proof, using the normalization condition, goes as below:

$$\delta(p_x - p'_x) = \langle p_x|p'_x\rangle = \int_{-\infty}^{\infty} \langle p_x|x\rangle \langle x|p'_x\rangle \, dx$$

$$= |N|^2 \int_{-\infty}^{\infty} \left(e^{-\imath \frac{p_x}{\hbar} x}\right) \left(e^{\imath \frac{p'_x}{\hbar} x}\right) dx$$

$$= |N|^2 \, 2\pi\hbar \; \delta(p_x - p'_x)$$

So we get that $N = 1/\sqrt{2\pi\hbar}$.

Expansion on momentum states (unbounded particle)

$$|\psi\rangle = \int dp_x c(p_x)|p_x\rangle, \quad \rightarrow \quad \psi(x) = \int_{-\infty}^{+\infty} dp_x c(p_x)\psi_{p_x}(x) \tag{4.24}$$

$dp_x|c(p_x)|^2$: Probability for momentum measurement in $(p_x, p_x + dp_x)$.

Thus we see that the quantity $|c(p_x)|^2$ is the *probability distribution* for the momentum measurements. At this point it arises the following problem; if we know the particle's wavefunction, $\psi(x)$ how it is possible to calculate $c(p_x)$? In this case we can immediately calculated the statistical properties of momentum measurements of particles such as, probabilities, averages and uncertainties. In the next paragraph we'll see that $c(p_x)$ is (simply) the Fourier Transformation (FT) of $\psi(x)$. For now we'll show this for the case of unbounded particles, but in any case the idea stands for the bounded case as well.

From $\psi_p(x)$ to $c(p)$. We take Eq. (4.24) and multiply from the left with $\psi^*_{p_{x'}}(x)$ and integrate over the space:

$$\begin{aligned}
\psi(x) &= \int_{-\infty}^{+\infty} dp_x c(p_x)\psi_{p_x}(x) \qquad \rightarrow \\
\int_{-\infty}^{+\infty} dx\psi^*_{p'_x}(x)\psi(x) &= \int_{-\infty}^{+\infty} dx\psi^*_{p'_x}(x)\left(\int_{-\infty}^{+\infty} dp_x c(p_x)\psi_{p_x}(x)\right) \\
&= \int_{-\infty}^{+\infty} dp_x c(p_x)\left(\int_{-\infty}^{+\infty} dx\psi^*_{p'_x}(x)\psi_{p_x}(x)\right) \\
&= \int_{-\infty}^{+\infty} dp_x c(p_x)\left(\langle\psi_{p_x}|\psi_{p'_x}\rangle\right) = \int_{-\infty}^{+\infty} dp_x c(p_x)\delta(p_x - p'_x) \\
&= c(p'_x)
\end{aligned}$$

Then we arrive at

$$c(p'_x) = \int_{-\infty}^{+\infty} dx\psi^*_{p'_x}(x)\psi(x) = \langle p'_x|\psi\rangle$$

We may now drop the 'prime' to simplify notation summarize our finding:

Momentum distribution of $\psi(x)$

$$c(p_x) = \langle p_x|\psi\rangle = \int_{-\infty}^{+\infty} dx\psi^*_{p_x}(x)\psi(x) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty} dx\psi(x)e^{-\imath\frac{p_x x}{\hbar}}, \tag{4.25}$$

in agreement with the claim that $c(p_x)$ is the FT of $\psi(x)$ (*change* $x/\hbar \to X$ *and the analogy is complete*). In any case one needs to perform an integration to switch from $\psi(x)$ to $c(p)$.

Quantum averages and Observables in position basis

At this point one can calculate quantum averages of any observable by considering the action of observables in the continuous position basis space. So assume a quantum observable which depends on the position and momentum observables, say,

$$\hat{Q} = \hat{Q}(\hat{X}, \hat{P}_x).$$

In order to find the average value of $\hat{Q}$ we can use the representation in the position basis, starting from the standard definition of the quantum average:

$$\left\langle \hat{Q} \right\rangle = \langle \psi | \hat{Q}(\hat{X}, \hat{P}_x) | \Psi \rangle = \int dx \psi^*(x) \hat{Q}(x, -\imath \frac{\partial}{\partial x}) \psi(x) \tag{4.26}$$

Average of the position observable (unbounded case).

Let's test the case of the $\hat{X}$ observable. Let's take the case of unbounded particle in state $|\psi\rangle$ described by a wavefunction $\psi(x)$. Its quantum average is for $\hat{Q} = \hat{X}$ gives,

$$\left\langle \hat{X} \right\rangle_\psi = \langle \psi | \hat{X} | \psi \rangle = \int dx \psi^*(x) x \psi(x) dx = \int dx x |\psi(x)|^2$$

For the case of $\hat{Q} = \hat{X}^2$ if we run the same procedure again:

$$\left\langle \hat{X}^2 \right\rangle_\psi = \int dx \psi^*(x) x^2 \psi(x) = \int dx x^2 |\psi(x)|^2.$$

With these two together we can calculate the uncertainty in the measurement of the average position as well, , since,

$$\langle \Delta \hat{X} \rangle_\psi = \sqrt{\left\langle \hat{X}^2 \right\rangle_\psi - \left\langle \hat{X} \right\rangle_\psi^2}$$

Average of the Momentum observable (unbounded case).

Let's test the case of the $\hat{P}_x$ observable Its quantum average is for $\hat{Q} = \hat{P}_x$ gives,

$$\left\langle \hat{P}_x \right\rangle_\psi = \langle \psi | \hat{P}_x | \psi \rangle = \int dx \psi^*(x) (-\imath\hbar \frac{d}{dx}) \psi(x) dx = -\imath\hbar \int dx \psi^*(x) \psi'(x)$$

For the case of $\hat{Q} = \hat{P}_x^2$ if we run the same procedure again:

$$\left\langle \hat{P}_x^2 \right\rangle_\psi = \int dx \psi^*(x) (-\imath\hbar \frac{d}{dx})^2 \psi(x) = -\hbar^2 \int dx \psi^*(x) \psi''(x). \tag{4.27}$$

With these two together we can calculate the uncertainty in the measurement of the average position as well, , since,

$$\langle \Delta \hat{P}_x \rangle_\psi = \sqrt{\langle \hat{P}_x^2 \rangle_\psi - \langle \hat{P}_x \rangle_\psi^2}$$

Example

A particle is confined 1-D region of space of length, L.

(a) What is the probability distribution density for this particle?

(b) What is it's wavefunction?

(c) What is the average of the position measurements and the uncertainty ?

Solution:

Let's set a 1-D coordinate system Ox. We set the origin at the middle of the interval, L. So, the particle can be found anywhere between, $-L/2$ and $L/2$ (Figure 4.2).

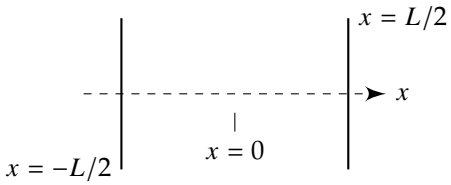


Figure 4.2

The particle is in a state $|\psi\rangle$ and it is associated with a wavefunction, $\psi(x) = \langle x|\psi\rangle$. Taking into account the statistical interpretation of $|\psi(x)|^2$ we have,

$$dx|\psi(x)|^2 = dP(x) = Prob\{x, x+dx\}, \quad \text{and} \quad \int_{-L/2}^{L/2} dx|\psi(x)|^2 = 1$$

But since there is no any preference where the particle maybe found upon position measurement we should assume that the probability density is as below,

$$\mathcal{P}(x) = \frac{dP(x)}{dx} = \begin{cases} C, & -L/2 \le x \le L/2, \\ 0 & \text{otherwise} \end{cases}$$

where C real positive number, $C > 0$. So we have,

$$\mathcal{P}(x) = |\psi(x)|^2 = C \qquad \rightarrow \qquad \rightarrow \qquad \psi(x) = e^{\imath\phi}\sqrt{C}$$

So the particle's wavefunction is a constant (since dx are considered of the same size at any position, x). This constant is determined by the normalization requirement:

$$\int_{-L/2}^{L/2} dx|\psi(x)|^2 = C^2 L = 1 \qquad \rightarrow \qquad C = \frac{1}{\sqrt{L}}.$$

Finally we have for the particle's wavefunction,

$$\psi(x) = \frac{1}{\sqrt{L}}, \qquad \mathcal{P}(x) = \frac{1}{L}, \quad dP(x) = \frac{dx}{L}.$$

The probability distribution density has units 1/length as expected and dP a dimensionless number (since it represents probability).

We want the average position in the x basis:

$$\langle \hat{X} \rangle = \langle \psi | \hat{X} | \psi \rangle = \int dx x |\psi(x)|^2 = \int_{-L/2}^{L/2} x \frac{1}{L} dx$$
$$= \frac{1}{L} \left(\frac{L^2}{4} - \frac{L^2}{4} \right) = 0.$$

We also need

$$\langle \hat{X}^2 \rangle = \langle \psi | \hat{X}^2 | \psi \rangle = \int dx x^2 |\psi(x)|^2 = \int_{-L/2}^{L/2} x^2 \frac{1}{L} dx$$
$$= \frac{1}{3L} \left(\frac{L^3}{8} - \frac{-L^3}{8} \right) = \frac{L^2}{12}.$$

So the uncertainty $\Delta X = \sqrt{\langle \hat{X}^2 \rangle}$ (since $\langle \hat{X} \rangle = 0$) is

$$\Delta X = \frac{L}{\sqrt{12}}. \tag{4.28}$$

Example

An particle has the following wavefunction:

$$\psi(x) = N \left(\frac{x}{L} \right) e^{-x^2/2L^2}, \qquad L > 0. \tag{4.29}$$

Calculate the the average position and the average momentum measurements.

Does this state satisfies the Heisenberg's uncertainty relations:

$$(\Delta \hat{X})_\psi (\Delta \hat{P}_x)_\psi \geq \frac{1}{2} |\langle [\hat{X}, \hat{P}_x] \rangle_\psi|$$

Solution:

First the wavefunction needs to be normalized, so that $|\psi(x)|^2 dx$ to represent probability distribution density, as required by QM. This is done via the normalization condition:

$$1 = \langle \psi | \psi \rangle = \int_{-\infty}^{\infty} |\psi(x)|^2 dx = \frac{|N|^2}{L^2} \int_{-\infty}^{\infty} x^2 e^{-x^2/L^2} dx = \frac{|N|^2 L \sqrt{\pi}}{2}$$

So our normalization constant is

$$N = \sqrt{\frac{2}{(L\sqrt{\pi})}}.$$

We now find average position:

$$\left\langle \hat{X} \right\rangle_\psi = \int dx x|\psi(x)|^2 = \frac{2}{L^3\sqrt{\pi}} \int dx x^3 e^{-x^2/L^2} = 0.$$

The average momentum is found by,

$$\left\langle \hat{P}_x \right\rangle_\psi = \int dx \psi^*(x)(-\imath\hbar \frac{d}{dx}\psi(x) = \cdots = 0.$$

where the $\cdots$ we're left to the reader to fill in.

Getting an average of zero for the position given the wavefunction distribution is reasonable. The momentum average zero indicates that the particle is moving in both directions with equal probability.

Let's now see the uncertainty relations.

We now know that $\left\langle \hat{X} \right\rangle = 0$ and $\left\langle \hat{P}_x \right\rangle = 0$. To find the uncertainties, we need $\left\langle \hat{X}^2 \right\rangle$ and $\left\langle \hat{P}_x^2 \right\rangle$:

$$\left\langle \hat{X}^2 \right\rangle_\psi = \frac{2}{L^3\sqrt{\pi}} \int_{-\infty}^{\infty} dx x^4 e^{-x^2/L^2} = \frac{3L^2}{2}$$

For the momentum's measurement uncertainty:

$$\begin{aligned}
\left\langle \hat{P}_x^2 \right\rangle_\psi &= \int dx \psi^*(x) \left(-\hbar^2 \frac{\partial^2}{\partial x^2} \right) \psi(x) \\
&= \frac{2}{L^3\sqrt{\pi}} \int_{-\infty}^{\infty} dx \; x e^{-x^2/2L^2} (-\hbar^2 \frac{\partial^2}{\partial x^2} \left(x e^{-x^2/2L^2} \right)) \\
&= \cdots = \frac{3\hbar^2}{2L^2}.
\end{aligned}$$

So the measurement uncertainties are

$$\begin{aligned}
(\Delta X)_\psi &= \sqrt{(\frac{3L^2}{2}) - 0^2} = \sqrt{\frac{3L^2}{2}} = L\sqrt{\frac{3}{2}} \\
(\Delta P_x)_\psi &= \sqrt{\frac{3\hbar^2}{2L^2} - 0^2} = \sqrt{\frac{3\hbar^2}{2L^2}} = \frac{\hbar}{L}\sqrt{\frac{3}{2}}.
\end{aligned}$$

The Heisenberg Uncertainty relationship is thus

$$(\Delta X)_\psi (\Delta P_x)_\psi = \frac{3}{2}\hbar > \frac{1}{2}|\langle [\hat{X}, \hat{P}_x] \rangle| = \frac{1}{2}|\langle \imath\hbar \rangle| = \frac{\hbar}{2}. \tag{4.30}$$

The state is in agreement with the Heisenberg's uncertainty relations.

The quantum harmonic oscillator

5

5.1 The classical simple harmonic oscillator

Let's consider a particle of mass m moving in a potential field of an harmonic oscillator. According to classical mechanics its potential energy outside its equilibrium position (assumed to be at $x = 0$) is $V(x) = m\omega_0 x^2/2$.

For a classical HO the equation of motion is and its solutions are,

$$\ddot{x}(t) + \omega_0^2 x(t) = 0$$

Defining $m\dot{x} = p(t)$ the above 2nd-order ODE is written as,

$$\dot{p}(t) = -m\omega_0^2 x(t)$$
$$\dot{x}(t) = p(t)/m$$

For a given set of initial conditions, $x(0) = x_0$ and $v(0) = v_0$ the solutions are,

$$x(t) = x_0 \cos\omega_0 t + \frac{p_0}{m\omega_0} \sin\omega_0 t = A_0 \sin(\omega_0 t + \phi_0)$$
$$p(t) = p_0 \cos\omega_0 t - m x_0 \omega_0 \sin\omega_0 t = m A_0 \cos(\omega_0 t + \phi_0)$$

Energy is *constant of motion* and equal to,

$$E = \frac{1}{2}mv^2 + \frac{1}{2}m\omega_0^2 x^2 = \frac{p^2}{2m} + \frac{1}{2}m\omega_0^2 x^2 = \frac{1}{2}m\omega_0^2 A_0^2 \qquad (5.1)$$

According to the above the energy of a simple HO is allowed to have any positive value and as such it represents a continuous quantity. We can also see that for the present frictionless HO for a given initial energy, say $E_0 = E(t = 0) > 0$, the motion of the particle is restricted to a certain range since,

$$v^2 = \frac{2E}{m} - \omega_0^2 x^2 > 0 \quad \rightarrow \quad -A_0 \le x \le A_0, \qquad A_0 = \sqrt{\frac{2E}{m\omega_0^2}}$$

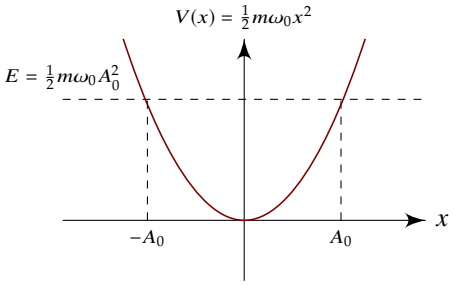


Figure 5.1: The potential energy diagram for a simple HO. Any value of energy, $E > 0$ is possible. Therefore, the energy takes continuous positive values.

5.2 The quantum harmonic oscillator (QHO)

The analogue of the quantum harmonic oscillator (QHO) is obtained as follows

(1) The starting point is the classical expression for the system's energy in terms of the momentum and position, which here is (5.1). The Hamiltonian is obtained by assuming that position and momentum are quantum observables, satisfying,

$$[\hat{x}, \hat{p}] = \imath\hbar,$$

Then the system's Hamiltonian is expressed by,

$$\hat{H}_{ho} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega_0^2\hat{x}^2. \tag{5.2}$$

The above expression for the Hamiltonian observable is given in the abstract algebraic formulation of QM.

(2) Second step is to choose a working representation for the $\hat{H}_{ho}$; here we choose the *position-representation* where the position- and the-momentum observables are expressed as below:

$$\hat{x} = x \qquad \hat{p} = -\imath\hbar\frac{d}{dx}. \tag{5.3}$$

By replacing expressions (5.3) into (5.2) we obtain:

$$H_{ho} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega_0^2x^2 \tag{5.4}$$

At this stage, it is obvious that the Hamiltonian in the position-representation becomes a differential operator with respect to the position, 'x'.

(3) In order to predict the outcome of the measurements of an arbitrary observable $\hat{Q}$ we need to determine the associated eigenvalues/eigenstates for the corresponding measured observable (e.g. energy, momentum, position,..).

(4) The dynamics of the system is given by the Schrödinger equation, [74]

$$\imath\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}_{ho}|\psi(t)\rangle \qquad \longrightarrow \qquad \imath\frac{\partial}{\partial t}\psi(x,t) = \hat{H}_{ho}\psi(x,t) \tag{5.5}$$

74: where, $\psi(x,t) = \langle x|\psi(t)\rangle$

5.3 HO eigenstates

Starting from the formal QM expression for eigenvalue problem of the Hamiltonian we arrive at the conclusion that the HO's spectrum is discretized and bounded from below. So, we have, [75]

$$\hat{H}_{ho}|\phi_n\rangle = E|\phi_n\rangle \qquad \Longrightarrow \qquad \hat{H}_{ho}\phi_n(x) = E\phi_n(x)$$

Substituting the HO hamiltonian (5.4) gives,

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega_0^2 x^2\right)\phi_n(x) = E_n\phi_n(x) \tag{5.6}$$

Defining,

$$\beta \equiv \sqrt{\frac{m\omega_0}{\hbar}} \tag{5.7}$$

the HO eigenfunctions and the corresponding eigenenergies are expressed as,

Harmonic oscillator spectrum

$$\phi_n(x) = N_n H_n(\beta x)e^{-\frac{1}{2}\beta^2 x^2}, \qquad E_n = \hbar\omega\left(n+\frac{1}{2}\right), \qquad n = 0,1,2,\cdots \tag{5.8}$$

$$\beta = \left(\frac{m\omega}{\hbar}\right)^{\frac{1}{2}}, \qquad N_n = \sqrt{\frac{\beta}{2^n n!\sqrt{\pi}}}$$

The QM orthonormalization and completeness relations for the $|\phi_n\rangle$,

$$\langle\phi_n|\phi_m\rangle = \delta_{nm} \qquad \mathbb{1} = \sum_n |\phi_n\rangle\langle\phi_n| \tag{5.9}$$

in the position representation the orthogonality condition become

$$\langle\phi_n|\phi_m\rangle = \int_{-\infty}^{\infty} dx\, \phi_n^*(x)\phi_m(x) = \delta_{nm} = \begin{cases} 1 & n = m \\ 0 & n \neq m. \end{cases} \tag{5.10}$$

$$\sum_n \phi_n(x)\phi(x') = \delta(x-x') \tag{5.11}$$

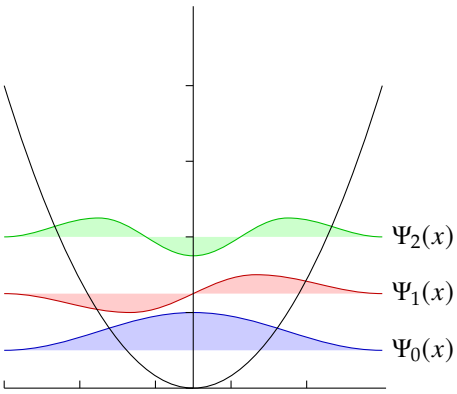
[76], We also see that any physical state (say $|\psi\rangle$) of the particle in the HO potential can be expressed in terms of the HO eigenstates. This can be seen by taking the completeness relation and by multiplying from the left to obtain,

$$|\psi\rangle = \sum_n |\phi_n\rangle\langle\phi_n|\psi\rangle = \sum_n c_n|\phi_n\rangle, \qquad c_n = \langle\phi_n|\psi\rangle \tag{5.12}$$

Now by assuming the position-representation, we can multiple again from the left with $\langle x|$ to obtain:

75: where, as usual

$$\phi_n(x) = \langle x|\phi_n\rangle$$
$$\hat{H}_{ho}\phi_n(x) = \langle x|\hat{H}_{ho}|\phi_n\rangle$$



76: To this the following properties of the position-eigenstates were used:

$$\int dx|x\rangle\langle x| = \mathbb{1}$$
$$\langle x|x'\rangle = \delta(x-x').$$

$$\psi(x) = \sum_n c_n \phi_n(x), \qquad c_n = \int_{-\infty}^{\infty} dx\, \phi_n^*(x)\psi(x), \tag{5.13}$$

where $\psi(x) = \langle x|\psi\rangle$ and $\phi_n = \langle x|\phi_n\rangle$.

5.4 Measurements

Measurement of an arbitrary observable $\hat{Q}$. In this case one should distinguish between the cases where the commutator $[\hat{Q}, \hat{H}]$ vanishes or not:

(i) $[\hat{Q}, \hat{H}] = 0$.
In this case the $|\phi_n\rangle$ are also eigenstates of $\hat{Q}$ and the following relation is true:

$$\hat{Q}|\phi_n\rangle = q_n|\phi_n\rangle \qquad \Longrightarrow \qquad \hat{Q}\phi_n(x) = q_n\phi_n(x)$$

[77]

(ii) $[\hat{Q}, \hat{H}] \neq 0$
Now it is required to solve the eigenvalue problem for $\hat{Q}$ and then to express the energy eigenstates in terms of the $\hat{Q}$ eigenstates (say $|q_n\rangle$). At this point one can extract information about the probability distribution of measurrements of the $\hat{Q}$ observable among its eigenvalues (which according to QM are the only one realized.)

77: Where Q is the representation of $\hat{Q}$ in the x-representation. One example of such operator is,

$$\begin{aligned}\hat{a} &= \frac{1}{\sqrt{2}}(x + \hat{p}) \\ &= \frac{1}{\sqrt{2}}(x - \imath\hbar\frac{d}{dx}).\end{aligned}$$

Energy measurement. The standard QM interpretation of the expansion coefficients, as the probability that an energy measurement will result to an eigenvalue E_n with probability:

$$P(E = E_n, t) = |c_n(t)|^2 = |c_n e^{-\imath\omega_0(n+1/2)}| = |c_n|^2. \qquad \textbf{(constant in time)}$$

Example: Probability, Mean value and standard deviation

Assume an HO quantum system ($V(x) = m\omega_0^2/2$) initially prepared in the state,

$$\psi_0 = \frac{1}{\sqrt{6}}(\phi_0 + 2\phi_1 + i\phi_4).$$

The *non-zero* expansion coefficients are

$$c_0 = \frac{1}{\sqrt{6}}, \quad c_1 = \frac{2}{\sqrt{6}}, \quad c_4 = \frac{\imath}{\sqrt{6}}$$

First one checks that the state is correctly normalized to unity:

$$\langle\psi_0|\psi_0\rangle = \sum_n |c_n|^2 = |c_0|^2 + |c_1|^2 + |c_4|^2 = 1.$$

Energy measurement will give the following results with the corresponding probabilities:

Energy	Probability
$E_0 = \frac{1}{2}\hbar\omega_0$	$P_0 = \lvert c_0\rvert^2 = \frac{1}{6}$
$E_1 = \frac{3}{2}\hbar\omega_0$	$P_1 = \lvert c_1\rvert^2 = \frac{2}{3}$
$E_4 = \frac{9}{2}\hbar\omega_0$	$P_4 = \lvert c_4\rvert^2 = \frac{1}{6}$

Note that, according to QM, if a measurement gives E_4, then the system's state immediately after measurement is ϕ_4. Of course a subsequent *energy* measurement will give E_4 with certainty.
The mean energy, $\langle\hat{H}\rangle$, in the initial state, ψ_0, may be evaluated as,

$$\langle\hat{H}\rangle_0 = \sum_n E_n |c_n|^2 = \left(\frac{1}{2}\cdot\frac{1}{6} + \frac{3}{2}\cdot\frac{2}{3} + \frac{9}{2}\cdot\frac{1}{6}\right)\hbar\omega_0 = \frac{11}{6}\hbar\omega_0.$$

To calculate the standard deviation, $\Delta H_0 = \sqrt{\langle\hat{H}^2\rangle_0 - \langle\hat{H}\rangle_0}$ one needs, in addition, to calculate $\langle\hat{H}^2\rangle$:

$$\langle\hat{H}^2\rangle_0 = \sum_n E_n^2 |c_n|^2 = \left((\frac{1}{2})^2\cdot\frac{1}{6} + (\frac{3}{2})^2\cdot\frac{2}{3} + (\frac{9}{2})^2\cdot\frac{1}{6}\right)(\hbar\omega_0)^2 = \frac{59}{12}(\hbar\omega_0)^2.$$

Therefore the standard deviation is,

$$\Delta H_0 = \hbar\omega_0\sqrt{\frac{59}{12} - (\frac{11}{6})^2} = \frac{\sqrt{14}}{3}\hbar\omega_0 \approx 1.247\hbar\omega_0.$$

Note: You may calculate the same quantities but for the state at a later time.

$$\psi(t) = \frac{1}{\sqrt{6}}(\phi_0 e^{-\imath\omega_0 t/2} + 2\phi_1 e^{-3\imath\omega_0 t/2} + i\phi_4 e^{-9\imath\omega_0 t/2}).$$

5.5 Dynamics of a particle in an HO potential

There are few different approaches to determine the relevant dynamics, depending on the available information. If the state of the system is known then one can calculate $\langle\hat{Q}\rangle$ directly. If the state of the system is known by its mean values then one could use the Ehrenfrest theorem. Or alternatively one could solve directly the time-dependent Schrödinger equation without relying in the knowledge of the eigenenergies/states. Let's discuss these approaches in a bit more detail.[78]

78: Note that the expectation (mean) value as the 'average result of many measurements' does not apply lightly for a QM system. Since, following a measurement, the system will end to one of its eigenstate, a subsequent measurement will give the corresponding eigenvalue with certainty. So, within QM the mean value is not practically obtained by measuring the same single system over many times. Instead, one performs the same type of measurement (once) on an number of identical copies of the same system prepared in the same state ψ. This is known as *ensemble* average

Evaluation of $\langle\hat{Q}\rangle$ and $\langle\Delta Q\rangle$

First one needs to calculate the time-evolution of an arbitrary state by expanding on the Hamiltonian's eigenstate basis:

$$|\psi\rangle = \sum_n c_n(0)|\phi_n\rangle \qquad \rightarrow \qquad |\psi(t)\rangle = \sum_n c_n(0)e^{-\imath E_n t/\hbar}|\phi_n\rangle \tag{5.14}$$

In the position representation by recalling (5.15) one has,

$$\psi(x,0) = \sum_n c_n\phi_n(x) \qquad \Longrightarrow \qquad \psi(x,t) = \sum_n c_n e^{-\imath\omega_0(n+1/2)}\phi_n(x). \tag{5.15}$$

Mean values For an arbitrary observable $\hat{Q}$ and when the particle is in an arbitrary state $|\psi(t)\rangle = \sum_n c_n|\phi_n\rangle$, QM gives for the expectation value (or mean value from a probabilistic point of view):

$$\langle\hat{Q}(t)\rangle_\psi = \langle\psi(t)|\hat{Q}|\psi(t)\rangle = \sum_{nm} c_n^*(0)c_m(0)e^{\imath(E_n-E_m)t/\hbar}Q_{nm}, \tag{5.16}$$

$$Q_{nm} = \langle\phi_n|\hat{Q}|\phi_m\rangle. \tag{5.17}$$

In the case of the HO (and again within the chosen position representation) the QM expression for mean values of observables (5.16) specializes to,

$$\langle\hat{Q}\rangle(t) = \langle\psi(t)|\hat{Q}|\psi(t)\rangle = \sum_{nm} c_n^* c_m e^{\imath\omega_0(n-m)t}Q_{nm}, \tag{5.18}$$

$$Q_{nm} = \int_{-\infty}^{\infty} dx\, \phi_n^*(x)\hat{Q}\phi_m(x) \tag{5.19}$$

Mean value of energy, $\langle\hat{H}\rangle$. For the special case of the energy mean value, $\hat{Q} = \hat{H}$, since $\hat{H}\phi_n(x) = E_n\phi_n(x)$ we end up to: [79]

$$H_{nm} = E_m\int_{-\infty}^{\infty} dx\, \phi_n^*(x)\phi_m(x) = E_m\delta_{nm} \qquad \rightarrow \qquad \langle H(t)\rangle = \sum_n E_n|c_n|^2$$

79: Which has the standard appearance of a (classical) mean value, $\langle E\rangle = \sum_n E_n P_n$, with $P_n = P(E = E_n)$ the probability distribution among energies E_n.

Mean value of position and momentum, $\langle\hat{x}\rangle$ and $\langle\hat{p}\rangle$. Let's specialize the above in the case of the classical mechanics dynamical variables, $\hat{x}$ and $\hat{p}$. From (5.18) and (5.19) it is seen that the matrix elements x_{nm} and p_{mn} over the HO energy eigenstates are needed for the calculation of $\langle\hat{x}\rangle$ and $\langle\hat{p}\rangle$ [80].

80: Or equivalently the expression of the $\hat{x}$ and $\hat{p}$ in the *energy*-representation, $|\phi_n\rangle$.

Fortunately, with the help of the properties of the Hermite polynomials these matrix elements can be calculated quite straightforward for arbitrary n and m:

(i)

$$x_{nm} = \langle\phi_n|\hat{x}|\phi_m\rangle = \int_{-\infty}^{\infty} dx\, \phi_n^*(x) x \phi_m(x) \tag{5.20}$$

(ii)

$$p_{nm} = \langle\phi_n|\hat{p}|\phi_m\rangle = \int_{-\infty}^{\infty} dx\, \phi_n^*(x)) \left(-\imath\frac{d}{dx}\right) \mathbf{1}\phi_m(x) \tag{5.21}$$

Example: Mean value, standard deviation of $\hat{x}$ in state $|\phi_n\rangle$

$$\begin{aligned}
\langle x\rangle_n = x_{nn} &= \int_{-\infty}^{\infty} dx\, \phi_n^*(x) x \phi_n(x) = \int_{-\infty}^{\infty} dx\, N_n e^{-\beta^2x^2/2} H_n(\beta x) x N_n e^{-\beta^2x^2/2} H_n(\beta x) = N_n^2 \int_{-\infty}^{\infty} dx\, x e^{-\beta^2x^2} H_n^2(\beta x) \\
&= \frac{N_n^2}{\beta^2}\left[\int_{-\infty}^{0} d(\beta x)\,(\beta x) e^{-(\beta x)^2} H_n^2(\beta x) + \int_{0}^{\infty} d(\beta x)\,(\beta x) e^{-(\beta x)^2} H_n^2(\beta x)\right] \\
&= \frac{N_n^2}{\beta^2}\left[\int_{-\infty}^{0} d(-\beta x)\,(-\beta x) e^{-(-\beta x)^2} [(-1)^n H_n(-\beta x)]^2 + \int_{0}^{\infty} d(\beta x)\,(\beta x) e^{-(\beta x^2)} H_n^2(\beta x)\right] \\
&= \frac{N_n^2}{\beta^2}\left[\int_{-\infty}^{0} du\, u e^{-u^2} H_n^2(u) + \int_{0}^{\infty} dv\, v e^{-v^2} H_n^2(v)\right] = \frac{N_n^2}{\beta^2}\left[-\int_{\infty}^{0} du\, u e^{-u^2} H_n^2(u) + \int_{0}^{\infty} dv\, v e^{-v^2} H_n^2(v)\right] = 0
\end{aligned}$$

since the last two integrals have the same value. Note that set $u = -\beta x$ and $v = \beta x$ and used the (parity) property of the Hermite polynomials $H_n(x) = (-1)H_n(-x)$. The standard deviation of is now given by

$$\Delta x_n = \sqrt{\langle x^2\rangle_n - \cancelto{0}{\langle x\rangle_n}} \qquad \rightarrow \qquad \Delta x_n = \sqrt{\langle x^2\rangle_n}$$

The calculation now proceeds along similar steps as for $\langle x\rangle_n$, to have,

$$\begin{aligned}
\langle x^2\rangle_n = x_{nn}^2 &= \int_{-\infty}^{\infty} dx\, \phi_n^*(x) x^2 \phi_n(x) = N_n^2 \int_{-\infty}^{\infty} dx\, x e^{-\beta^2x^2} H_n^2(\beta x) = \frac{N_n^2}{\beta^2}\int_{-\infty}^{+\infty} dx\, e^{-\beta^2x^2} (\beta x H_n(\beta x))^2 \\
&= \frac{N_n^2}{\beta^2}\int_{-\infty}^{+\infty} dx\, e^{-\beta x^2}\left(\frac{1}{2}H_{n+1}^2(\beta x) + nH_{n-1}(\beta x)\right)^2 = \frac{N_n^2}{\beta^2}\int_{-\infty}^{+\infty} dx\, e^{-\beta x^2}\left[\frac{1}{4}H_{n+1}^2(\beta x) + n^2H_{n-1}^2(\beta x) + nH_{n+1}(\beta x)H_{n-1}(\beta x)\right] \\
&= \frac{N_n^2}{\beta^2}\int_{-\infty}^{+\infty} dx\, e^{-\beta^2x^2}\left[\frac{1}{4N_{n+1}^2}N_{n+1}^2H_{n+1}^2(\beta x) + \frac{n^2}{N_{n-1}^2}N_{n-1}^2H_{n-1}^2(\beta x) + \frac{n}{N_{n+1}N_{n-1}}N_{n+1}H_{n+1}(\beta x)N_{n-1}H_{n-1}(\beta x)\right] \\
&= \frac{1}{\beta^2}\left[(\frac{N_n}{2N_{n+1}})^2 \cancelto{1}{\langle\phi_{n+1}|\phi_{n+1}\rangle} + (\frac{nN_n}{N_{n-1}})^2 \cancelto{1}{\langle\phi_{n-1}|\phi_{n-1}\rangle} + \frac{nN_n}{N_{n+1}N_{n-1}} \cancelto{0}{\langle\phi_{n+1}|\phi_{n-1}\rangle}\right] = \frac{1}{\beta^2}\left[(\frac{N_n}{2N_{n+1}})^2 + (\frac{nN_n}{N_{n-1}})^2\right] \\
&= \frac{1}{\beta^2}\left[\frac{n+1}{2} + \frac{n}{2}\right] = \frac{1}{\beta^2}(n+\frac{1}{2}) = \frac{\hbar}{m\omega_0}(n+\frac{1}{2}) = \frac{E_n}{m\omega_0^2}.
\end{aligned}$$

To perform the above integrals the following relations were used,

$$xH_n(x) = H_{n+1}(x) + nH_{n-1}(x), \qquad \langle\phi_n|\phi_m\rangle = \delta_{nm}, \qquad N_n = \sqrt{\frac{\beta}{2^n n!\sqrt{\pi}}}$$

Finally we end up to following general properties for an HO in its eigenstate:

$$\langle x\rangle_n = 0, \qquad \langle x^2\rangle_n = \frac{E_n}{m\omega_0^2} \qquad \Delta x_n = \sqrt{\frac{E_n}{m\omega_0^2}} \tag{5.22}$$

Example: Mean value, standard deviation of $\hat{p}$ in the HO state $|\phi_n\rangle$.

For the mean value of the momentum we have $\langle p\rangle_n$, to have,

$$\begin{aligned}
\langle p\rangle_n &= \hat{p}_{nn} = \int_{-\infty}^{\infty} dx\, \phi_n^*(x)\hat{p}\phi_n(x) = N_n^2 \int_{-\infty}^{\infty} dx\, e^{-\beta^2x^2/2} H_n(\beta x)(-\imath\hbar\frac{d}{dx})\left[e^{-\beta^2x^2/2}H_n(\beta x)\right] \\
&= N_n^2 \int_{-\infty}^{\infty} dx\, e^{-\beta^2x^2/2} H_n(\beta x)\left[\imath\hbar x\beta^2 e^{-\beta^2x^2/2}H_n(\beta x) - \imath\hbar\beta e^{-\beta^2x^2/2}\frac{d}{d(\beta x)}H_n(\beta x)\right] \\
&= \imath\hbar\int_{-\infty}^{\infty} dx\, xN_n^2\beta^2 e^{-\beta^2x^2}H_n^2(\beta x) - \imath\hbar\beta\int_{-\infty}^{\infty} dx\, N_n e^{-\beta^2x^2/2}H_n(\beta x)e^{-\beta^2x^2/2}\,[2nH_{n-1}(\beta x)] \\
&= \imath\hbar\,\cancelto{0}{\langle\phi_n|x|\phi_n\rangle} - 2\imath\hbar\beta\frac{2n}{N_{n-1}}\int_{-\infty}^{\infty} dx\,\left(N_n e^{-\beta^2x^2/2}H_n(\beta x)\right)\left(N_{n-1}e^{-\beta^2x^2/2}H_{n-1}(\beta x)\right) \\
&= -2\imath\hbar\beta\frac{2n}{N_{n-1}}\,\cancelto{0}{\langle\phi_n|\phi_{n-1}\rangle} = 0
\end{aligned}$$

To perform the above integrals the following relations were used,

$$\frac{d}{dx}H_n(\beta x) = \beta\frac{d}{d(\beta x}H_n(\beta x) = \beta H'(u) = \beta 2nH_{n-1}(u) = 2n\beta H_{n-1}(\beta x) \quad \rightarrow \quad \frac{d}{dx}H_n(\beta x) = 2n\beta H_{n-1}(\beta x) \qquad \langle\phi_n|\phi_{n-1}\rangle = 0,$$

The standard deviation of the mean value is now given by,

$$\Delta p_n = \sqrt{\langle\hat{p}^2\rangle_n - \cancelto{0}{\langle\hat{p}\rangle_n}} \quad \rightarrow \quad \Delta p_n = \sqrt{\langle\hat{p}^2\rangle_n}$$

For the calculation of the required $\langle \text{op}^2\rangle$ we can go ahead along the way already presented. Alternatively, at this point we can take advantage of the Hamiltonian expression for the HO in terms of $\langle\hat{x}^2\rangle$ and $\langle\hat{p}^2\rangle$. So using (5.2) we have,

$$\langle\hat{p}^2\rangle = 2m\langle\hat{H}\rangle - m^2\omega_0^2\langle x^2\rangle = 2mE_n - m^2\omega_0^2\frac{E_n}{m\omega_0^2} = mE_n, \tag{5.23}$$

where the mean value of $\langle\hat{x}^2\rangle$ used from (5.24) and that $\langle H\rangle = E_n$.

Finally we end up to following general properties for an HO in its eigenstate:

$$\langle p\rangle_n = 0, \qquad \langle p^2\rangle = mE_n, \qquad \Delta p_n = mE_n = \sqrt{mE_n}, \tag{5.24}$$

Based on the above results we can also evaluate the Heisenberg's relation for an HO in the state $|\phi_n\rangle$:

$$\Delta x_n\Delta p_n = \sqrt{\frac{E_n}{m\omega_0^2}}\sqrt{mE_n} = \frac{E_n}{\omega_0} = \hbar(n+\frac{1}{2}). \tag{5.25}$$

81

81: Therefore the uncertainty relation takes its minimum value when the system is in its ground state ($\phi_0(x)$):

$$\Delta x_0\Delta p_0 = \frac{\hbar}{2}$$

Equation of motion (EOM) for $\langle\hat{Q}\rangle$

To simplify the discussion we'll consider the Ehrenfrest theorem for observables that are not dependent on time explicitly [82] . Examples of such observables are the usual operators such as the position, momentum, energy, etc.. Then we have,

82: So

$$\frac{\partial\hat{Q}}{\partial t} = 0.$$

$$\imath\hbar\frac{d}{dt}\langle\hat{Q}\rangle = \langle[\hat{Q},\ \hat{H}_{ho}]\rangle\frac{1}{2m}\langle[\hat{Q},\ \hat{p}^2]\rangle + \frac{1}{2}m\omega_0^2\langle[\hat{Q},\ \hat{x}^2]\rangle.$$

From the above we see that the commutation relations $[\hat{p},\ \hat{Q}]$ and $[\hat{x},\ \hat{Q}]$ are required in order to establish the EOM for $\langle\hat{Q}\rangle$. At this point

one needs to know the explicit expression for

EOMs for $\langle\hat{x}\rangle$ and $\langle\hat{p}\rangle$. As an example, we can specialize and try to find the equations of motions for the mean values of $\hat{x}$ and $\hat{p}$. This is done as below,

$$\imath\hbar\frac{d}{dt}\langle\hat{x}\rangle = \langle[\hat{x},\ \hat{H}_{ho}]\rangle = \langle[\hat{x},\ \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega_0^2\hat{x}^2]\rangle = \frac{1}{2m}\langle[\hat{x},\ \hat{p}^2]\rangle + \frac{1}{2}m\omega_0^2\langle[\hat{x},\ \hat{x}^2]\rangle$$
$$\imath\hbar\frac{d}{dt}\langle\hat{p}\rangle = [\hat{p},\ \hat{H}_{ho}] = \langle[\hat{p},\ \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega_0^2\hat{x}^2]\rangle = \frac{1}{2m}\langle[\hat{p},\ \hat{p}^2]\rangle + \frac{1}{2}m\omega_0^2\langle[\hat{p},\ \hat{x}^2]\rangle$$

Now, using $[\hat{x},\ \hat{p}] = \imath\hbar$ by noting that

$$[\hat{x},\ \hat{x}^2] = [\hat{p},\ \hat{p}^2] = 0,$$
$$[\hat{x},\ \hat{p}^2] = 2\imath\hbar\hat{p},$$
$$[\hat{p},\ \hat{x}^2] = -2\imath\hbar\hat{x},$$

resulting to,

$$[\hat{x},\ \hat{H}_{ho}] = \imath\hbar\frac{\hat{p}}{m}, \qquad [\hat{p},\ \hat{H}_{ho}] = -\imath\hbar m\omega_0^2\hat{x}.$$

The final EOM then become, [83]

$$\frac{d}{dt}\langle\hat{x}\rangle = \frac{\langle\hat{p}\rangle}{m}$$
$$\frac{d}{dt}\langle\hat{p}\rangle = -m\omega_0^2\langle\hat{x}\rangle$$

83: The first equation resembles the classical definition of momentum while the second one the equation of motion for the classical simple HO (after replacing $\frac{d}{dt}\langle\hat{x}\rangle = \langle\hat{p}\rangle$) :

$$\frac{d^2}{dt^2}\langle\hat{x}\rangle + \omega_0^2\langle\hat{x}\rangle = 0.$$

So given the mean values of the system's momentum and position at some time (say $t_0 = 0$) the corresponding solutions are,

$$\langle x\rangle(t) = x_0\cos\omega_0 t + \frac{p_0}{m\omega_0}\cos\omega_0 t, \qquad x_0 = \langle x\rangle(0) \tag{5.26}$$
$$\langle p\rangle(t) = p_0\cos\omega_0 t - m\omega_0 x_0\sin\omega_0 t, \qquad p_0 = \langle p\rangle(0) \tag{5.27}$$

Therefore the classical equations of motion are still valid in the quantum case, however for the corresponding expectation values! [84]

84: Nevertheless this reminiscinent of the classical motion it is only true if the HO's state is NOT an eigenstate. Then its behaviour is uniquely quantum!

5.6 Solution of the HO eigenvalue equation*

[85] The objective in this section is to provide the solution procedure for the HO's eigenvalue equation (). We have,

$$\begin{aligned}
&\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{1}{2}m\omega_0^2x^2\right)\phi(x)=E\phi(x),\\
\rightarrow\quad &\frac{d^2\phi(x)}{dx^2}-\left[(\frac{m\omega_0}{\hbar})^2\,x^2-\frac{2mE}{\hbar^2}\right]\phi(x)=0,\\
\rightarrow\quad &\frac{d^2\phi(x)}{dx^2}-\frac{m\omega_0}{\hbar}\left[\frac{m\omega_0}{\hbar}\,x^2-\frac{2E}{\hbar\omega_0}\right]\phi(x)=0\\
\rightarrow\quad &\frac{d^2\phi(x)}{d(\beta x)^2}-\left[(\beta x)^2-\frac{2E}{\hbar\omega_0}\right]\phi(x)=0,
\end{aligned}$$

where the β parameter (5.7) was introduced [86]. At this stage is convenient to introduce the scaled variables, X and $\mathscr{E}$ we end up to,

$$X=\left(\frac{m\omega_0}{\hbar}\right)^{\frac{1}{2}}x=\beta x,\qquad \mathscr{E}=\frac{E}{\hbar\omega},\tag{5.28}$$

both of which is dimensionless. Then we are left with

$$\phi''(X)-(X^2-2\mathscr{E})\phi(X)=0,\tag{5.29}$$

with the differentiation with respect to X. This DE requires one more variable transformation before we end up to a familiar (in mathematical physics) DE. So the following transformation is introduced [87],

$$\Phi(X)=h(X)e^{-\frac{1}{2}X^2}.\tag{5.30}$$

Then the Schrödinger equation gives,

$$\boxed{h''(X)-2Xh'(X)+(2\mathscr{E}-1)=0.}\tag{5.31}$$

This is known as *Hermite's equation* a well-studied differential equation in the 19th century [88]

The series expansion and the normalization condition. A typical method of solving DEs with constant coefficients is to assume a power expansion of the solution in terms of the independent variable (here is X) with the task to find the unknown expansion coefficients:

$$h(X)=\sum_r c_rX^r,\qquad r=0,1,\cdots.$$

Direct substitution into the Hermite's equation gives,

$$\sum_{r\geq 0}\left[(r+2)(r+1)c_{r+2}+(2\mathscr{E}-1-2r)c_r\right]X^r=0.$$

In order the above to be true for all powers it is required that,

$$\frac{c_{r+2}}{c_r}=\frac{2r+1-2\mathscr{E}}{(r+2)(r+1)}\qquad r\geq 0.$$

85: *Not necessary for the final exams

86:
$$\beta=\sqrt{\frac{m\omega_0}{\hbar}}$$

87: The rationale for this change goes as follows: For large X, such that $X^2\gg\mathscr{E}$ the term $\mathscr{E}\phi(X)$ cannot offset $X^2\phi(X)\rightarrow\infty$. Therefore the DE will blow up, unless the $\phi''(X)$ term is of the same order as the $X^2\phi(X)$ term. The second derivative of a Gaussian exponential ($\sim e^{-X^2}$) produces down a factor X^2 and behaves as $\sim -X^2e^{-X^2}$.

88: Named after Charles Hermite (French, 1822-1902) despite that first were introduced by Pierre Simon Laplace in 1810 and later studies in detail by P. L. Chebyshev in 1859.

Note that that this recursive expression relates coefficients which differ by 2 in their index. So two independent solutions are derived one including only even powers and the other only odd powers. Therefore this method gives the two independent solutions required from a 2nd-order differential equations.

From a physical point of view the expansion series cannot be of 'infinite order' since then the solution (again) will explode for large X. Simple inspection shows that the series terminates for some $r = n$ such that

$$2n + 1 - 2\mathscr{E} = 0 \quad \rightarrow \quad \mathscr{E}_n = n + \frac{1}{2}$$

$$\rightarrow \quad \boxed{E_n = \hbar\omega_0(n + \frac{1}{2}), \quad n = 0, 1, 2, ..}$$

The latter relation gives the (now) quantized energies, E_n. For any given $n = 0, 1, 2..$ the expansion solution is now given by, [89]

$$H_n(X) = \sum_r^n 2c_r \frac{r - n}{(r + 2)(r + 1)} X^r, \qquad r = \begin{cases} 0, 2, \cdots, n & \text{n even} \\ 1, 3, \cdots, n & \text{n odd} \end{cases} \tag{5.32}$$

In the above it was assumed $c_0 = 1$ and $c_1 = 1$ (chosen independently) to get two linearly independent solutions. For example, we have

$$H_0(X) = c_0$$
$$H_1(X) = c_1 X$$
$$H_2(X) = c_0(1 - 2X^2)$$
$$H_3(X) = c_1\left(X - \frac{2}{3}X^3\right).$$

These are known as the *Hermite polynomials*. [90] By combining (5.30) and (5.32) we obtain the HO eigenfunctions as ,

$$\phi_n(x) = N_n H_n(\beta x) e^{-\beta^2 x^2/2} \tag{5.33}$$

with a slight change of notation ($\Phi_n(X) = \Phi_n(\beta x) = \phi_n(x)$.

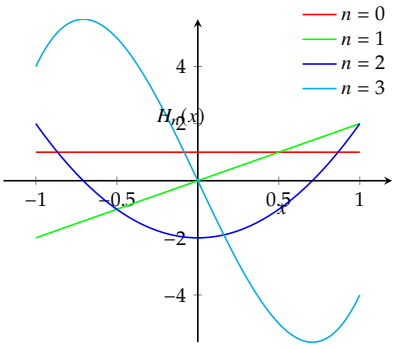


Figure 5.2: The graph of some Hermite polynomials.

89: Note the change of notation $h(X) \rightarrow H_n(X)$ to emphasize that one is restricted to Hermite polynomials H_n.

90: There are numerous relations for the Hermite polynomials easily found in the print and digital literature. For our purposes and for the *normalized* $H_n(x)$ the following hold:

$$H_0(x) = 1, \qquad H_1(x) = 2x$$
$$H_2(x) = 4x^2 - 2, \quad H_3(x) = 8x^3 - 12x$$
$$\delta_{nm}(2^n n!\sqrt{\pi}) = \int_{-\infty}^{\infty} dx\, e^{-x^2} H_n(x) H_m(x)$$
$$H_n(-x) = (-1)^n H_n(x)$$
$$H_n'(x) = 2nH_{n-1}(x),$$
$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x)$$
$$H_{n+1}(x) = 2xH_n(x) - H_n'(x)$$

5.7 Tutorial problems

(1) **Virial theorem**. In classical mechanics for a particle moving in a potential energy field of the form $V(x) = ax^n$ the following relation holds for the time-average of the total kinetic and potential energy:

$$\langle T\rangle_t = \frac{n}{2}\langle V\rangle_t, \qquad V(x) = ax^n. \tag{5.34}$$

This is known as *Virial theorem*.
(a) Specialize the above virial theorem for a particle of mass m ib the case of a classical HO.
(b) Show that for a particle in an quantum HO potential energy and in its eigenstate the following relations hold the mean values,

$$\langle T\rangle_n = \langle V\rangle_n = \frac{E_n}{2} \tag{5.35}$$

(2) **Explicit calculations for the low-energy states.** Consider the ground and the first excited state of a particle in an HO potential (m, ω_0). By explicit calculations of the relevant integrals: [91]
(a) Show that $\langle\hat{x}\rangle_0 = \langle\hat{x}\rangle_1 = 0$ and that $\langle\hat{p}\rangle_0 = \langle\hat{p}\rangle_1 = 0$
(b) Calculate the (dipole) matrix elements x_{01} and p_{01}
(The results compatible with the general expressions given in the main text.)

91: You can use the following Gaussian Integrals:

$$\int_{-\infty}^{\infty} dx e^{-ax^2} = \sqrt{\frac{\pi}{a}},$$
$$\int_{0}^{\infty} dx\, x e^{-ax^2} = \frac{1}{2a},$$
$$\int_{-\infty}^{\infty} dx\, x^2 e^{-ax^2} = \frac{1}{2a}\sqrt{\frac{\pi}{a}},$$

(3) **Matrix elements of $\hat{x}$, $x_{nn'}$.**
(a) Use the properties of the Hermite polynomials to show that,

$$\hat{x}\phi_n(x) = \sqrt{\frac{\hbar}{2m\omega_0}}\left[\sqrt{n+1}\phi_n(x) + \sqrt{n}\phi_{n-1}(x)\right] \tag{5.36}$$

(b) Using the above calculate the arbitrary (dipole) matrix elements:

$$x_{nn'} = \langle\phi_n|\hat{x}|\phi_{n'}\rangle = ? \tag{5.37}$$

(4) **Matrix elements of** op**, $p_{nn'}$.**
(a) Use the properties of the Hermite polynomials to show that,

$$\hat{p}\phi_n(x) = \sqrt{\frac{m\omega_0}{2\hbar}}\left[\sqrt{n+1}\phi_n(x) - \sqrt{n}\phi_{n-1}(x)\right] \tag{5.38}$$

(b) Using the above calculate the arbitrary (dipole) matrix elements:

$$p_{nn'} = \langle\phi_n|\hat{p}|\phi_{n'}\rangle = ? \tag{5.39}$$

(5) **Harmonic oscillator in an electric field** Assume a particle of mass m and charge q, subject to an HO potential and and a constant electric field of amplitude $\mathscr{E}_0$. Therefore the potential energy of the particle is,

$$V(x) = \frac{1}{2}m\omega_0 x^2 + q_m\mathscr{E}_0\, x$$

(a) Provide an expression of its Hamiltonian in the position representation
(b) Assume that the particle is initially at a state where its mean position and momentum are zero. Using the Heisenber relations

show that the corresponding mean values are time-dependent given by,

$$\langle x\rangle(t) = \frac{q\mathscr{E}_0}{m\omega_0^2}(1-\cos\omega_0 t) \qquad \langle p\rangle(t) = \frac{q\mathscr{E}_0}{\omega_0}\sin\omega_0 t \tag{5.40}$$

(c) Give the energy mean value $\langle H\rangle$.

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*: In the questions we name as *fundamental* basis,

$$|1\rangle = \begin{pmatrix}1\\0\\0\end{pmatrix}, \qquad |2\rangle = \begin{pmatrix}0\\1\\0\end{pmatrix} \qquad |3\rangle = \begin{pmatrix}0\\0\\1\end{pmatrix}$$

and 2-D fundamental basis:

$$|1\rangle = \begin{pmatrix}1\\0\end{pmatrix}, \qquad |2\rangle = \begin{pmatrix}0\\1\end{pmatrix}$$

CA1 Question 1 **(30 Marks)**

Consider a quantum system in the state (i.e. a molecule in a particular rotational state):

$$|\psi\rangle = N|q_1\rangle + \frac{\imath}{2}|q_2\rangle - \frac{1}{\sqrt{2}}|q_3\rangle,$$

expressed in the eigenbasis of an observable $\hat{L}$. In this basis the matrix-reprsentation of the observable is expressed as,

$$\hat{L} = \begin{pmatrix}-\hbar & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & \hbar\end{pmatrix} \tag{6.1}$$

where $\hbar$ is the reduced Planck's constant, $\hbar = h/2\pi$.

(a) Find N so that $|\psi\rangle$ is normalized to unity.
(b) If we measure $\hat{L}$ what are the possible values and with what probability?
(c) In this state find the average of the results, $\langle L\rangle_\psi$ and the uncertainty of the measurements, $(\Delta L)_\psi$?

Solution **(a)** QM states owe to be normalized to unity. This requirements will determine an acceptable value for N [93] :

$$\langle\psi|\psi\rangle = |N|^2 + |\frac{\imath}{2}|^2 + |-\frac{1}{\sqrt{2}}|^2 = 1 \qquad \rightarrow \qquad |N|^2 = \frac{1}{4} \rightarrow \boxed{N_\phi = \frac{e^{\imath\phi}}{2}}.$$

Note that here we cannot ignore the phase factor $e^{\imath\phi}$ because it has physical significance For example, take the states corresponding to the choices $\phi = 0$, $\phi = \pi/2$ or $\phi = \pi$ are the below:

$$|\psi\rangle_{\phi=0} = \frac{1}{2}|q_1\rangle + \frac{\imath}{2}|q_2\rangle - \frac{1}{\sqrt{2}}|q_3\rangle,$$
$$|\psi\rangle_{\phi=\frac{\pi}{2}} = \frac{\imath}{2}|q_1\rangle + \frac{\imath}{2}|q_2\rangle - \frac{1}{\sqrt{2}}|q_3\rangle,$$
$$|\psi\rangle_{\phi=\pi} = -\frac{1}{2}|q_1\rangle + \frac{\imath}{2}|q_2\rangle - \frac{1}{\sqrt{2}}|q_3\rangle,$$

These are physically different each other, since they lead to different predictions about measurement of physical quantities. So we end up

93: The phase factor has *no physical significance* if and only if appears as a common factor (or global factor) to all terms of the expansion relation. For example, for the case where the state had be given as,

$$|\psi'\rangle = N'\left(|q_1\rangle + \frac{\imath}{2}|q_2\rangle - \frac{1}{\sqrt{2}}|q_3\rangle\right)$$

In this case, $|N'|^2 = 4/7$ and:

$$N'_\phi = e^{\imath\phi}\sqrt{\frac{4}{7}} \qquad \rightarrow \qquad N'_0 = \sqrt{\frac{4}{7}}$$

The special choice $\phi_0 = 0$ is fully legitimated according to QM as it doesn't lead to any different physical predictions had we chosen any other value of ϕ. In other words, once more the expressions,

$$e^{\imath\phi}\sqrt{\frac{4}{7}}\left(|q_1\rangle + \frac{\imath}{2}|q_2\rangle - \frac{1}{\sqrt{2}}|q_3\rangle,\right)$$
$$\sqrt{\frac{4}{7}}\left(|q_1\rangle + \frac{\imath}{2}|q_2\rangle - \frac{1}{\sqrt{2}}|q_3\rangle,\right)$$

maybe used equally to represent the state $|\psi'\rangle$.

to the following representation for $|\psi\rangle$ in terms of $|q_i\rangle, i = 1-3$:

$$\boxed{|\psi\rangle = \frac{e^{\imath\phi}}{2}|q_1\rangle + \frac{\imath}{2}|q_2\rangle - \frac{1}{\sqrt{2}}|q_3\rangle} \tag{6.2}$$

(b) Since $|q_i\rangle,\ i = 1-3$ are eigenstates of $\hat{L}$ we have,

$$\hat{L}|q_i\rangle = q_i|q_i\rangle, \qquad i = 1,2,3.$$

Let's take, $|q\rangle_i$ to be the fundamental basis $|i\rangle$ such that

$$|q\rangle_i \equiv |i\rangle, \qquad i = 1-3.$$

Then we have, for example for $i = 1$:

$$\hat{L}|q_1\rangle = \hat{L} = \begin{pmatrix} -\hbar & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \hbar \end{pmatrix}\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = -\hbar\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = -\hbar|q_1\rangle = q_1|q_1\rangle$$

Doing the same for the other two states $|q_2\rangle, |q_3\rangle$ we eventually find that,

$$q_1 = -\hbar, \qquad q_2 = 0, \qquad = +\hbar.$$

Now by direct interpretation of the given superposition expansion in terms $|q\rangle_1$ [Eq. (6.2)] we can calculate the results of the $\hat{L}$ measurements and their appearance probability as [94] :

$$\begin{aligned} P_1 = P(\hat{L} = -\hbar) &= |\langle q_1|\psi\rangle|^2 = |c_1|^2 = |\frac{e^{\imath\phi}}{2}|^2 = \frac{1}{4} \\ P_2 = P(\hat{L} = 0) &= \cdots = \frac{1}{4} \\ P_3 = P(\hat{L} = -\hbar) &= \cdots = \frac{1}{2}. \end{aligned}$$

94: Recall the QM postulate 1:

$$|\psi\rangle = \sum_{q=1-3} c_i\,|q_i\,\rangle, \qquad c_i = \langle q_1|\psi\rangle.$$

(c)

It is straightforward to calculate the average of $\hat{L}$ by a variety of methods. If we choose the statistical approach very quickly we obtain [95] :

$$\langle\hat{L}\rangle_\psi = \sum_{i=1-3} P_i q_i = \frac{1}{4}\times(-\hbar) + \frac{1}{4}\times(0) + \frac{1}{2}\times(\hbar) = \boxed{\frac{\hbar}{4}}.$$

95: or using the QM definition:

$$\langle\hat{L}\rangle_\psi = \langle\psi|\hat{L}|\psi\rangle.$$

Similarly for the measurements of $\hat{L}^2$:

$$\langle\hat{L}^2\rangle_\psi = \sum_{i=1-3} P_i q_i^2 = \frac{1}{4}\times(-\hbar)^2 + \frac{1}{4}\times(0) + \frac{1}{2}\times(\hbar)^2 = \frac{3\hbar^2}{4}.$$

From the above we have for the uncertainty:

$$(\Delta\hat{L})_\psi = \sqrt{\langle\hat{L}^2\rangle_\psi - \langle\hat{L}\rangle_\psi^2} = \sqrt{\frac{3\hbar^2}{4} - (\frac{\hbar}{4})^2} = \boxed{\frac{\hbar}{4}\sqrt{11}.}$$

Note: We notice here that the phase factor $e^{\imath\phi}$ played no role in the QM predictions about the measurements of $\hat{L}$. In other words, regard-

less the choice of ϕ we would have arrived at the same results about probabilities P_i, averages and uncertainties of $\hat{L}$ measurements. However this should not mislead us as this conclusion holds true only for observables that have $|q_i\rangle$ as eigenstates, that is for those that are commuting with $\hat{L}$, $[\hat{L}, \hat{Q}] = 0$.

Relative phase factors in a linear superposition expansion.

The relative phases in a linear superposition expansion of a state play no role for observables which have $|q\rangle_i$ as eigenstates. The significance of the relative phases in the eigen-expansion emerges for observables that do not have the $|q_i\rangle$ as eigenstates.

CA1 Question 2 **(30 Marks)**

Suppose at an atom is initially in the state,

$$|\psi_0\rangle = \frac{1}{2}|1\rangle + \imath\frac{\sqrt{3}}{2}|2\rangle, \tag{6.3}$$

with a Hamiltonian matrix in this basis ($\hbar\omega_0 = 10.277$ eV):

$$\hat{H} = \begin{pmatrix} \hbar\omega_0/2 & 0 \\ 0 & -\hbar\omega_0/2 \end{pmatrix}$$

(a) What are the possible values that can be obtained if energy measurements take place?
(b) Calculate $|\psi(t)\rangle$ at times $t_k = k\pi/\omega_0,\ k = 1/2, 1, 3/2, 2$
(c) At time $t = \pi/\omega_0$ calculate the average energy and its uncertainty value in eV and find the characteristic time evolution of the atom's statistical properties in seconds.

Solution: **(a)** This problem is very similar with the previous one, with the difference that now the dimension of the observable is 2 instead of 3. The eigenstate expansion of the state $|\psi\rangle$ is given together with the observable which now is the system's Hamiltonian[96]. Furthermore the state is properly normalized:

96: This means that we can find the state evolution of the system using the Schrödinger Equation.

$$\langle\psi_0|\psi_0\rangle = |\frac{1}{2}|^2 + |\imath\frac{\sqrt{3}}{2}|^2 = \frac{1}{4} + \frac{3}{4} = 1.$$

So, (assuming the fundamental basis $|1\rangle, |2\rangle$,for energy measurements we have

$$P_1 = P(\hat{H} = \frac{\hbar\omega_0}{2}) = |\langle 1|\psi_0\rangle|^2 = |c_1|^2 = |\frac{1}{2}|^2 = \frac{1}{4}$$
$$P_2 = P(\hat{H} = -\frac{\hbar\omega_0}{2}) = |\langle 2|\psi_0\rangle|^2 = |c_2|^2 = |\imath\frac{\sqrt{3}}{2}|^2 = \frac{3}{4}$$

(b)

Since the state $|\psi_0\rangle$ is expanded on the Hamiltonian's eigenstates it its simple matter to know how it evolves in time by simply adding the energy-phase factors in the respective amplitudes, according the rule

$$|\psi_0\rangle = \sum_i c_i|E_i\rangle \qquad \rightarrow \qquad |\psi_t\rangle = \sum_i c_i e^{-\imath\frac{E_i t}{\hbar}}|E_i\rangle$$

Here, $|E_i\rangle \equiv |i\rangle$ and $E_1 = \hbar\omega/2, E_2 = -\hbar\omega_0/2$. Therefore we have,

$$|\psi(t)\rangle = \frac{1}{2}e^{-\imath\frac{E_1 t}{\hbar}}|1\rangle + \imath\frac{\sqrt{3}}{2}e^{-\imath\frac{E_2 t}{\hbar}}|2\rangle = \frac{1}{2}e^{-\imath\omega_0 t/2}|1\rangle + \imath\frac{\sqrt{3}}{2}e^{\imath\omega_0 t/2}|2\rangle$$

Now the state at the times $t_k = k\pi/\omega_0$ for $k = 1/2, 1, 3/2, 2$ are calculated easily.

(**c)** In particular the state at time $t' = \pi/\omega_0$,

$$|\psi'\rangle = \frac{e^{-\imath\pi/2}}{2}|1\rangle + \imath\frac{e^{\imath\pi/2}\sqrt{3}}{2}|2\rangle = \boxed{-\frac{1}{2}|1\rangle + \imath\frac{\sqrt{3}}{2}|2\rangle}$$

The average energy as usual maybe calculated by using the statistical definition of an average:

$$E = \langle\hat{H}\rangle = \sum_i P_i E_i = \cdots = |-\frac{1}{2}|^2 \times (\frac{\hbar\omega_0}{2}) + |\imath\frac{\sqrt{3}}{2}|^2 \times (\frac{-\hbar\omega_0}{2}) = \frac{\hbar\omega_0}{2}(-\frac{1}{4} + \frac{3}{4}) = \frac{\hbar\omega_0}{4}$$

Similarly,

$$E^2 = \langle\hat{H}^2\rangle = \sum_i P_i E_i = \cdots = |-\frac{1}{2}|^2 \times (\frac{\hbar\omega_0}{2})^2 + |\imath\frac{\sqrt{3}}{2}|^2 \times (\frac{-\hbar\omega_0}{2})^2 = (\frac{\hbar\omega_0}{2})^2(\frac{1}{4} + \frac{3}{4}) = (\frac{\hbar\omega_0}{2})^2$$

Eventually we obtain for the uncertainty of the energy measurements:

$$(\Delta\hat{H})_\psi = \sqrt{\langle\hat{H}^2\rangle_\psi - \langle\hat{H}\rangle_\psi^2} = \sqrt{(\frac{\hbar\omega_0}{2})^2 - (\frac{\hbar\omega_0}{4})^2} = \boxed{\hbar\omega_0\frac{\sqrt{3}}{4}.}$$

CA1 Question 3 **(30 Marks)**

The matrix-representation of the Hamiltonian of a quantum system in the fundamental basis $|1\rangle, |2\rangle$

$$\hat{H} = E_0 \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \qquad E_0 > 0,$$

The system is in the state

$$|\psi\rangle = |2\rangle$$

Upon measurement of the energy of this system find:

(a) The possible energy values

(b) the probability that the energy measurement will give the lowest possible value.

Solution: (a)

This problem has been solved in the case where the system is initially at $|1\rangle$ (see Question **??**) The part (a) follows exactly the same lines are in this question.

(b) *Measurement of energy*.

Here one should follow the same reasoning but for the state $|2\rangle$. The expansion of the state $|2\rangle$ in terms of the Hamiltonian's eigenstates $|\phi_1\rangle$ (with eigenvalue $\epsilon_1 = -E_0\sqrt{2}$) and $|\phi_2\rangle$ (with eigenvalue $\epsilon_1 = +E_0\sqrt{2}$) (see Eq. (2.51) [97]:

$$|2\rangle = \left(-\frac{1}{2}\sqrt{2+\sqrt{2}}\right)|\phi_1\rangle + \left(\frac{1}{2}\sqrt{2-\sqrt{2}}\right)|\phi_2\rangle.$$

Since the eigestate $|\phi_1\rangle$ has as an eigenvalue $\epsilon_1 = -E_0\sqrt{2}$ an energy measurement will give this value with probability,

$$P_1(E = -\frac{E_0}{\sqrt{2}}) = |c_1|^2 = \left|-\frac{1}{2}\sqrt{2+\sqrt{2}}\right|^2 = \boxed{\frac{2+\sqrt{2}}{4}},$$

97: Or re-written as,

$$P_1(E<0) = \frac{2+\sqrt{2}}{4} = \frac{(\sqrt{2}+1)}{2\sqrt{2}} = \frac{(\sqrt{2}+1)(\sqrt{2}+1)}{2\sqrt{2}(\sqrt{2}+1)} = \frac{1}{2}\frac{(\sqrt{2}+1)^2}{(2+\sqrt{2})}$$

CA1 Question 4 **(10 Marks)**

Given the representation of the observables, $\hat{A}$ and $\hat{B}$ in the fundamental basis, $|1\rangle, |2\rangle, |3\rangle$:

$$\hat{A} = a\begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}, \qquad \hat{B} = b\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{6.4}$$

Calculate $(\Delta\hat{A})_\psi$, $(\Delta\hat{B})_\psi$ and $|\langle[\hat{A}, \hat{B}]\rangle_\psi|$. Also, confirm the uncertainty relation for the product $(\Delta A)_\psi(\Delta B)_\psi$, when

(a) $|\psi\rangle = |1\rangle$

(b)

$$|\psi\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ \imath \end{pmatrix}$$

Solution: To calculate the uncertainties for the measurements of $\hat{A}$ and $\hat{B}$ we need to calculate, $\langle\hat{A}\rangle$, $\langle\hat{A}^2\rangle$ and $\langle\hat{B}\rangle$, $\langle\hat{B}^2\rangle$. Then we have from the general QM expression for averages:

$$\langle\hat{Q}\rangle_\psi = \langle\psi|\hat{Q}|\psi\rangle$$

(a) Let's assume the system is in the state $|\psi\rangle = |1\rangle$.

Then for $\hat{Q} = \hat{A}$ we get,

$$\langle\hat{A}\rangle_1 = \langle 1|\hat{A}|1\rangle = \underbrace{\begin{pmatrix} 1, 0, 0 \end{pmatrix}}_{\langle 1|} \cdot \underbrace{a\begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}}_{\mathbf{A}} \cdot \underbrace{\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}}_{|1\rangle} = a,$$

and for $\hat{Q} = \hat{A}^2$:

$$\hat{A}^2 = \hat{A} \cdot \hat{A} = a\begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix} a\begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix} = a^2\begin{pmatrix} 1 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 4 \end{pmatrix}.$$

We then immediately get,

$$\langle\hat{A}^2\rangle_1 = \langle 1|\hat{A}^2|1\rangle = \underbrace{\begin{pmatrix} 1, 0, 0 \end{pmatrix}}_{\langle 1|} \cdot \underbrace{a^2\begin{pmatrix} 1 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 4 \end{pmatrix}}_{\mathbf{A}} \cdot \underbrace{\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}}_{|1\rangle} = a^2$$

Uncertainty (standard deviation) The standard deviation of the measurements of an observable $\hat{Q}$ when the system is in state $|\psi\rangle$ is,

$$(\Delta Q)_\psi = \sqrt{\langle\psi|(\hat{Q} - \langle Q\rangle_\psi)^2|\psi\rangle} = \sqrt{\langle\mathbb{Q}^2\rangle_\psi - \langle\mathbb{Q}\rangle_\psi^2}. \tag{6.5}$$

Replacing $\hat{Q}$ by $\hat{A}$ and using $|\psi\rangle = |1\rangle$ we find

$$(\Delta A)_1 = \sqrt{\langle \hat{A}^2 \rangle_1 - \langle \hat{A} \rangle_1^2} = \sqrt{a^2 - a^2} = 0 \tag{6.6}$$

Summarizing we have for the the $\hat{A}$ in the state $|1\rangle$

Statistical measurements for $\hat{A}$ in state $|1\rangle$

$$\langle A \rangle_1 = a, \qquad (\Delta \hat{A})_1 = 0.$$

In fact this is something that we should have expected by noticing that $\hat{A}$ is diagonal and $|1\rangle$. This means that $|1\rangle$ is also an eigenstate of $\hat{A}$ with eigenvalue a:

$$\hat{A}|1\rangle = a \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = a \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = a|1\rangle \qquad \rightarrow \qquad \hat{A}|1\rangle = a|1\rangle$$

Therefore we have a system in an eigenstate ($|1\rangle$) of the observable $\hat{A}$. Then measurements of $\hat{A}$ will give with certainty the eigenvalue of this eigenstate (here a). So, uncertainty is expected to be zero!. Following the same lines of thinking let's evaluate the action of $\hat{B}$ (which is non-diagonal) on $|1\rangle$:

$$\hat{B}|1\rangle = b \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = b \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = b|2\rangle \qquad \rightarrow \qquad \hat{B}|1\rangle = b|2\rangle$$

In other words the state $|1\rangle$ is not an eigenvalue of $\hat{B}$ since:

$$\hat{B}|1\rangle \neq (\text{some real number}) \times |1\rangle.$$

Nevertheless measurements of $\hat{B}$ can still be provided via the QM rules but now there is an associated uncertainty which is non-zero. So following the standard procedure we have, for $\hat{Q} = \hat{B}$ we get,

$$\langle \hat{B} \rangle_1 = \langle 1|\hat{B}|1\rangle = \underbrace{\begin{pmatrix} 1, 0, 0 \end{pmatrix}}_{\langle 1|} \cdot \underbrace{b \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}}_{\mathbf{B}} \cdot \underbrace{\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}}_{|1\rangle} = \begin{pmatrix} 1, 0, 0 \end{pmatrix} \cdot b \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = 0,$$

and for $\hat{Q} = \hat{B}^2$:

$$\hat{B}^2 = \hat{B} \cdot \hat{B} = b \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} b \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} = b^2 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

The we calculate:

$$\langle \hat{B}^2 \rangle_1 = \langle 1|\hat{B}^2|1\rangle = \underbrace{\begin{pmatrix}1,0,0\end{pmatrix}}_{\langle 1|} \cdot \underbrace{b^2 \begin{pmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{pmatrix}}_{\mathbf{B}} \cdot \underbrace{\begin{pmatrix}1\\0\\0\end{pmatrix}}_{|1\rangle} = b^2$$

The uncertainty $(\Delta \hat{B})_1$ is now

$$(\Delta B)_1 = \sqrt{\langle \hat{B}^2 \rangle_1 - \langle \hat{B} \rangle_1^2} = \sqrt{b^2 - 0} = b$$

Summarizing we have for the the $\hat{B}$ in the state $|1\rangle$

Statistical measurements for $\hat{B}$ in state $|1\rangle$

$$\langle B \rangle_1 = 0, \qquad (\Delta \hat{B})_1 = b.$$

The result is that the mean value of the measurements of $\hat{B}$, when the system is in state $|1\rangle$ is zero, but the uncertainty is equal to b!

We know need to check the Heisenberg's uncertainty relation. [98] In our case we have calculated $(\Delta \hat{A})_1, (\Delta \hat{B})_1$ so it remains to calculate the right-hand-side of the inequality, that is the mean-value of the commutator $[\hat{A}, \hat{B}]$:

98: Which states,

$$(\Delta \hat{A})_\psi (\Delta \hat{B})_\psi \geq \frac{1}{2} |\langle [\hat{A}, \hat{B}] \rangle_\psi|$$

$$\hat{A} \cdot \hat{B} = a \begin{pmatrix}1 & 0 & 0\\ 0 & 2 & 0\\ 0 & 0 & 2\end{pmatrix} b \begin{pmatrix}0 & 1 & 0\\ 1 & 0 & 0\\ 0 & 0 & 1\end{pmatrix} = ab \begin{pmatrix}0 & 1 & 0\\ 4 & 0 & 0\\ 0 & 0 & 4\end{pmatrix}$$

and

$$\hat{B} \cdot \hat{A} = b \begin{pmatrix}0 & 2 & 0\\ 1 & 0 & 0\\ 0 & 0 & 1\end{pmatrix} a \begin{pmatrix}1 & 0 & 0\\ 0 & 2 & 0\\ 0 & 0 & 2\end{pmatrix} = ab \begin{pmatrix}0 & 1 & 0\\ 1 & 0 & 0\\ 0 & 0 & 2\end{pmatrix}.$$

The commutator then is,

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{A}\hat{B} = ab \begin{pmatrix}0 & 0 & 0\\ 3 & 0 & 0\\ 0 & 0 & 2\end{pmatrix}$$

and its mean value in state $|1\rangle$:

$$\langle [\hat{A}, \hat{B}] \rangle_1 = \langle 1|[\hat{A}, \hat{B}]|1\rangle = \begin{pmatrix}1,0,0\end{pmatrix} ab \begin{pmatrix}0 & 0 & 0\\ 3 & 0 & 0\\ 0 & 0 & 2\end{pmatrix} \begin{pmatrix}1\\0\\0\end{pmatrix} = 0.$$

Then from the uncertainty relation we have

$$(\Delta \hat{A})_1 (\Delta \hat{B})_1 \geq \frac{1}{2} |\langle [\hat{A}, \hat{B}] \rangle_1| \qquad \rightarrow \qquad 0 \times b \geq 0$$

which is fulfilled!

(b) For this subquestion one needs to repeat the above procedure but replacing $|1\rangle$ with $|\psi\rangle$. I let the reader to test the level of understanding and skills developed at this point.

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CA2 Question 1 **(25 Marks)**

Assume an electron moving freely ($V(x) = 0$) in the state,

$$\psi(x) = \frac{N}{x^2 + a^2}$$

(a) Calculate N and the mean values $\langle x \rangle, \langle p \rangle$.

(b) Calculate the probability that a position measurement will find the particle in the region $[-a, a]$.

(c) Calculate the probability that a momentum measurement will give a value between $[-\hbar/a, +\hbar/a]$

[hint: Use $\int_{-\infty}^{+\infty} dx \frac{\cos(kx)}{x^2+1} = \pi e^{-|k|}$.]

Solution:

(a) First $\psi(x)$ requires normalization:

$$\begin{aligned}\langle \psi | \psi \rangle = \int dx |\psi(x)|^2 = \int dx |\frac{N}{x^2 + a^2}|^2 = 1 \\ \rightarrow |N|^2 \int dx \frac{1}{(x^2 + a^2)^2} = |N|^2 \frac{\pi}{2a^3} \\ \rightarrow N = \sqrt{\frac{2a^3}{\pi}}\end{aligned}$$

where a global phase factor $e^{\imath\phi}$ in the normalization constant was ignored. We have for the wavefunction,

$$\psi(x) = \sqrt{\frac{2a^3}{\pi}} \frac{1}{x^2 + a^2}$$

For the mean values of the position and momentum we have,

$$\langle x \rangle = \int_{-\infty}^{+\infty} dx \psi^*(x) x \psi(x) = \int_{-\infty}^{+\infty} dx x |\psi(x)|^2 = \frac{2a^3}{\pi} \int_{-\infty}^{+\infty} dx \frac{x}{(x^2 + a^2)^2} = 0$$

since $f(x) = x/(x^2 + a^2)$ is odd function (antisymmetric, $f(x) = -f(-x)$). Also,

$$\langle p \rangle = \int_{-\infty}^{+\infty} dx \psi^*(x) (-\imath\hbar \frac{d}{dx}) \psi(x) = \int_{-\infty}^{+\infty} dx \psi(x) \psi'(x) = \imath\hbar \frac{2a^3}{\pi} \int_{-\infty}^{+\infty} dx \frac{2x}{(x^2 + a^2)^2} = 0,$$

100: The expression, eigenstates/eigenenergies of the position ($\hat{x}$), momentum ($\hat{p}$), free-Hamiltonian ($\hat{H}_f = \hat{p}^2/2m$) and harmonic oscillator ($\hat{H}_{ho} = \hat{p}^2/2m + m\omega_0^2\hat{x}^2/2$)-observables in the position-representation of a particle of mass m are as below,

$$\begin{aligned}\hat{x} = x, \quad \phi_{x'}(x) = \delta(x - x'), \\ \hat{x}\phi_{x'} = x\phi_{x'}, \quad \langle x | x' \rangle = \delta(x - x') \\ \hat{p} = -\imath\hbar \frac{d}{dx}, \\ \phi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{\imath p x/\hbar}, \quad \hat{p}\phi_p(x) = p\phi_p(x) \\ \hat{H}_f = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2}, \\ \phi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{\imath p x/\hbar}, \quad \hat{H}_f \phi_p(x) = \frac{p^2}{2m} \phi_p(x) \\ \hat{H}_{ho} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m\omega_0^2 x^2, \\ \phi_n(x) = N_n e^{-\beta^2 x^2/2} H_n(\beta x), \\ \hat{H}_{ho}\phi_n(x) = \hbar\omega_0 (n + \frac{1}{2}) \phi_n(x), \quad n = 0, 1, 2, \cdots \\ \beta = \sqrt{\frac{m\omega_0}{\hbar}}, \qquad H_n(x) \text{ Hermite polyn.},\end{aligned}$$

for that $2x/(x^2+a^2)$ is even function of x. Summarizing,

$$\boxed{N=\sqrt{\frac{2a^3}{\pi}}, \qquad \langle x\rangle = 0, \qquad \langle p\rangle = 0.}$$

(**b)** The probability for the position measurement is calculated by,

$$P(-a\le x\le a) = \int_{-a}^{a} dx|\psi(x)|^2 = \frac{2a^3}{\pi}\int_{-a}^{a} dx\frac{1}{(x^2+a^2)^2} = ??$$

(c) This is a more delicate question. One needs to advice the discussion prior to Eq. (4.25). We have a particle in state $\psi(x)$. We also know the eigenstate of momentum with eigenvalue p [101] :

$$\psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}}e^{\imath px/\hbar}$$

Then according to QM the probability [102] that a momentum measurement will give a value between $p, p+dp$ is,

$$P_\psi(\hat{p}\in(p,p+dp)) = dp = dp|\langle p|\psi\rangle|^2$$

then for the asked probability:

$$P_\psi(-\hbar/a\le p\le \hbar/a) = \int_{-\hbar/a}^{\hbar/a} dp\ |c(p)|^2 \tag{7.1}$$

So one has to calculate first the inner product $\langle p|\psi\rangle$:

$$\begin{aligned} c(p) = \langle p|\psi\rangle &= \int_{-\infty}^{+\infty} dx\phi_p^*(x)\psi(x) = \int_{-\infty}^{+\infty} dx\psi(x)\frac{e^{-\imath px/\hbar}}{\sqrt{2\pi\hbar}} \\ &= \sqrt{\frac{2a^3}{\pi}}\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty} dx\frac{1}{x^2+a^2}e^{\imath px/\hbar}, \\ &= \frac{a}{\pi}\sqrt{\frac{a}{\hbar}}\int_{-\infty}^{+\infty} dx\frac{1}{x^2+a^2}e^{\imath px/\hbar} \end{aligned}$$

The last integral is nothing else than the Fourier transform (FT) of $1/(x^2+a^2)$. This is calculated by setting $p=\hbar k$ and $X=x/a$ followed by expansion of the complex exponent as,

$$\begin{aligned} \int_{-\infty}^{+\infty} dx\frac{e^{-\imath px/\hbar}}{x^2+a^2} &= \frac{1}{a}\int_{-\infty}^{+\infty} d(\frac{x}{a})\frac{e^{\imath ka\frac{x}{a}}}{(\frac{x}{a})^2+1} = \frac{1}{a}\int_{-\infty}^{+\infty} dX\frac{e^{\imath kaX}}{(X^2+1} \\ &= \frac{1}{a}\left[\int_{-\infty}^{+\infty} dX\frac{\cos(kaX)}{X^2+1} + \imath\int_{-\infty}^{+\infty} dX\frac{\sin(kaX)}{X^2+1}\right] \\ &= \frac{1}{a}\left(\pi e^{-|ka|}+\imath 0\right) = \frac{\pi}{a}e^{-\frac{|p|a}{\hbar}} \end{aligned}$$

where the imaginary part vanishes on the basis that is a symmetric integration of an anti-symmetric $(\sin(kaX)/(X^2+1)$ function ($f(x)=$

101: We drop the index x from p_x as it is assumed that for this 1-D problem the coordinate axis is denoted by x.

102: Since $\psi(x) = \int_{-\infty}^{+\infty} dpc(p)\phi_P(x)$

$-f(-x)$)). Combining all the above Eventually we have for $c(p)$:

$$c(p) = \sqrt{\frac{a}{\hbar}} e^{-\frac{|p|a}{\hbar}} = \begin{cases} \sqrt{\frac{a}{\hbar}} e^{-\frac{pa}{\hbar}} & p > 0 \\ \sqrt{\frac{a}{\hbar}} e^{+\frac{pa}{\hbar}} & p < 0. \end{cases} \tag{7.2}$$

Now we are ready to calculate the requested probability. From (7.1),

$$\begin{aligned} P(-\frac{\hbar}{a} \leq p \leq \frac{\hbar}{a}) &= \int_{-\hbar/a}^{\hbar/a} dp|c(p)|^2 = \frac{a}{\hbar} \int_{-\hbar/a}^{\hbar/a} dp e^{-2\frac{|p|a}{\hbar}} \\ &= \frac{a}{\hbar} \left[\int_{-\hbar/a}^{0} dp e^{2\frac{pa}{\hbar}} + \int_{0}^{\hbar/a} dp e^{-2\frac{pa}{\hbar}} \right] \\ &= \frac{a}{\hbar} 2 \int_{0}^{\hbar/a} dp e^{-2\frac{pa}{\hbar}} = \frac{2a}{\hbar} \left[\frac{e^{-2pa/\hbar}}{-\frac{2a}{\hbar}} \right]_{0}^{\hbar/a} = \left(e^{0} - e^{-2} \right) = 1 - e^{-2} \end{aligned}$$

Finally,

$$\boxed{P(-\frac{\hbar}{a} \leq p \leq \frac{\hbar}{a}) = 1 - e^{-2} \simeq 0.864665}$$

CA2 Question 2 **(25 Marks)**

An electron is moving in the field of an infinite potential well of size L, with ground state energy $E_1 = 0.01$ eV.

$$\psi(x,0) = N\left[\phi_1(x) - \imath\phi_2(x)\right], \qquad \phi_1, \phi_2 \text{ eigenstates.}$$

(a) Find the particle's mean position and momentum values at time $t = 0$. Find the corresponding mean values at a later time $t = \hbar\pi/(2E_1)$.

(b) find the standard deviations Δx and Δp initially and at the later time $t = \hbar\pi/(2E_1)$. What is the value $\Delta x \Delta p$? Is this value consistent with Heisenberg's uncertainty relation?

Solution:

Here we need to use the infinite well eigenfunctions $\phi_n(x)$ [103] First we must properly normalize the wavefunction. At this point we use the fact that the infinite-well eigenfunctions are real to write,

$$|\psi(x,0)|^2 = |N|^2|\phi_1 - \imath\phi_2|^2 = |N|^2(|\phi_1|^2 + |\phi_2|^2) = |N|^2(\phi_1^2 + \phi_2^2).$$

We also have from the orthonormalization conditions for the eigenfunctions,

$$\int_0^L dx\phi_1^2(x) = \int_0^L dx\phi_2^2(x) = 1, \qquad \int_0^L dx\phi_1(x)\phi_2(x) = 0$$

Then, the normalization condition for $\psi(x)$ gives[104]:

$$\begin{aligned} 1 = \langle\psi|\psi\rangle &= \int_{-\infty}^{+\infty} dx|\psi(x,0)|^2 = |N|^2 \int_{-\infty}^{+\infty} dx|\phi_1(x) - \imath\phi_2(x)|^2 \\ &= |N|^2\left(\int_0^L dx\phi_1^2(x) + \int_0^L dx\phi_2^2(x)\right) = |N|^2(1+1) = 2|N|^2 \end{aligned}$$

So ignoring the global phase factor we have $N = 1/\sqrt{2}$ and for the wavefunction $\psi(x,0)$

$$\begin{aligned} \psi(x,0) &= \frac{1}{\sqrt{2}}\left[\phi_1(x) - \imath\phi_2(x)\right] \\ &= \frac{1}{\sqrt{L}}\left[\sin(\frac{\pi x}{L}) - \imath\sin(\frac{2\pi x}{L})\right] \end{aligned} \tag{7.3}$$

It's time evolution according the QM principles is then given by,

$$\psi(x,t) = \frac{1}{\sqrt{2}}\left[e^{-\imath\frac{E_1 t}{\hbar}}\phi_1(x) - e^{-\imath\frac{E_2 t}{\hbar}}\imath\phi_2(x)\right] = \frac{e^{-\imath\frac{E_1 t}{\hbar}}}{\sqrt{2}}\left[\phi_1(x) - e^{-\imath\frac{(E_2-E_1)t}{\hbar}}\imath\phi_2(x)\right]$$

Then we can ignore the global phase factor[105] $e^{-\imath\frac{E_1 t}{\hbar}} = e^{-\imath\theta}$ and defining

$$\omega_0 = \frac{E_2 - E_1}{\hbar}$$

103: **Infinite well eigenfunctions** $(0 \le x \le L)$

$$\phi_n(x) = \sqrt{\frac{2}{L}}\sin(\frac{n\pi x}{L}),$$
$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}, \qquad n = 1, 2, \cdots$$
$$\langle\phi_n|\phi_m\rangle = \int_0^L dx\phi_n(x)\phi_m(x) = \delta_{nm}.$$

104: We also have,

$$\phi_1(x) = \sqrt{\frac{2}{L}}\sin(\frac{\pi x}{L}), \quad E_1 = \frac{\pi^2\hbar^2}{2mL^2}$$
$$\phi_2(x) = \sqrt{\frac{2}{L}}\sin(\frac{2\pi x}{L}) \quad E_2 = 4\frac{\pi^2\hbar^2}{2mL^2} = 4E_1$$

105: For the same reason that we ignore phase factors for the normalization constants. They bear no physical significance

we may finally write for $\psi(x,t)$.

$$\psi(x,t) = \frac{1}{\sqrt{2}}\left[\phi_1(x) - \imath e^{-\imath\omega_0 t}\phi_2(x)\right] \tag{7.4}$$
$$= \frac{1}{\sqrt{L}}\left[\sin(\frac{\pi x}{L}) - \imath e^{-\imath\omega_0 t}\sin(\frac{2\pi x}{L})\right]$$

while its probability distribution density is (after some algebraic manipulations):

$$|\psi(x,t)|^2 = \frac{1}{2}\left[\phi_1^2(x) + \phi_2^2(x) + 2\phi_1(x)\phi_2(x)\sin(\omega_0 t)\right] \tag{7.5}$$
$$= \frac{1}{L}\left[\sin^2(\frac{\pi x}{L}) + \sin^2(\frac{2\pi x}{L}) + 2\sin(\frac{\pi x}{L})\sin(\frac{2\pi x}{L})\sin(\omega_0 t)\right]$$

Now that we know fully both $\psi(x,t)$ we can calculate any probability and average we are requested. Here we can use directly $\psi(x,t)$ and then set $t = 0$ to find the corresponding quantity at time $t = 0$. However for educational reasons I'll sketch the answers for $t = 0$ and let you to apply for $t > 0$.

(a) Mean position and momentum values require the calculation of the following relations:

$$\langle\hat{x}\rangle_0 = \langle\psi_0|\hat{x}|\psi_0\rangle = \int_0^L dx x|\psi(x)|^2 = \frac{1}{2}\int_0^L dx x|\phi_1(x) - \imath\phi_2(x)|^2$$
$$= \frac{1}{2}\left(\int_0^L dx x|\phi_1(x)|^2 + \int_0^L dx x|\phi_2(x)|^2\right)$$
$$= \int_0^L dx x\sin^2(\frac{\pi x}{L}) + \int_0^L dx x\sin^2(\frac{2\pi x}{L}) = \cdots =$$
$$= \frac{L}{4} + \frac{L}{4} = \boxed{\frac{L}{2}}$$

Generally one can prove that [106]

$$\langle x\rangle_1 = \langle\phi_1|x|\phi_1\rangle = \frac{L}{2}, \qquad \langle x\rangle_2 = \langle\phi_2|x|\phi_2\rangle = \frac{L}{2}.$$

Similar considerations hold for the momentum averages (for brevity we write $\psi(x,0) = \psi(x)$) [107] :

$$\langle\hat{p}\rangle_0 = \langle\psi_0|\hat{p}|\psi_0\rangle = \int_0^L dx\psi^*(x)\left(-\imath\hbar\frac{d}{dx}\right)\psi(x) = -\imath\hbar\int_0^L dx\psi^*(x)\psi'(x)$$
$$= -\imath\frac{\pi\hbar}{L^2}\int_0^L dx\left[\sin(\frac{\pi x}{L}) + \imath\sin(\frac{2\pi x}{L})\right]\left[\cos(\frac{\pi x}{L}) - 2\imath\cos(\frac{2\pi x}{L})\right]$$
$$= \frac{\pi\hbar}{L^2}\left[\int_0^L dx\sin(\frac{2\pi x}{L})\cos(\frac{\pi x}{L}) - 2\int_0^L dx\cos(\frac{2\pi x}{L})\sin(\frac{\pi x}{L})\right]$$
$$- \imath\frac{\pi\hbar}{L^2}\left[\int_0^L dx\sin(\frac{\pi x}{L})\cos(\frac{\pi x}{L}) + 2\int_0^L dx\sin(\frac{2\pi x}{L})\cos(\frac{2\pi x}{L})\right]$$
$$= \frac{\pi\hbar}{L^2}\left[\frac{4L}{3\pi} - 2(-\frac{2L}{3\pi})\right] - \imath\frac{\pi\hbar}{L^2}[0+0] = \boxed{\frac{8\hbar}{3L}}$$

So we may summarize for the initial average values,

106: It helps the evaluation if one uses the following identities:

$$\int_0^L dx\sin(\frac{n\pi x}{L})\sin(\frac{m\pi x}{L}) = \frac{L}{2}\delta_{nm},$$
$$\int_0^L dx\sin(\frac{n\pi x}{L})\cos(\frac{m\pi x}{L}) = 0$$

107: where the space derivative of $\psi(x)$ is,

$$\psi'(x,0) = \frac{\pi}{L\sqrt{L}}\left[\cos(\frac{\pi x}{L}) - \imath 2\cos(\frac{2\pi x}{L})\right]$$

average initial position and momentum values

$$\langle \hat{x} \rangle_0 = \frac{L}{2} \qquad \langle \hat{p} \rangle_0 = \frac{8\hbar}{3L}$$

For the corresponding averaged values one has to use the time-dependent wavefunction evaluated in (7.4). In this case one should expect to find [108]:

average initial position and momentum values at time t

$$\langle \hat{x} \rangle_t = \frac{L}{2} + \frac{16L}{9\pi^2} \sin(\omega_0 t) \tag{7.6}$$

$$\langle \hat{p} \rangle_t = \frac{8\hbar}{3L} \cos(\omega_0 t), \tag{7.7}$$

$$\omega_0 = \frac{3E_1}{\hbar} = \frac{3\pi^2\hbar}{2mL^2}$$

We then see that the particle 'oscillates' about the middle of the well with a period determined by the energy difference of the states ϕ_1 and ϕ_2. Similar oscillations occurs for the average momentum of the particle. Oscillates about zero with the same frequency.

Now, one can easily find the averages for $t_1 = \pi\hbar/2E_1$ to find,

$$\langle \hat{x} \rangle_{t_1} = \frac{L}{2} + \frac{16L}{9\pi^2} \sin(\omega_0 t_1) = \frac{L}{2} + \frac{16L}{9\pi^2} \sin(\frac{3\pi}{2}) = \frac{L}{2} - \frac{16L}{9\pi^2} \simeq \boxed{0.32L},$$

and

$$\langle \hat{p} \rangle_{t_1} = \frac{8\hbar}{3L} \cos(\omega_0 t_1) = \frac{8}{3\hbar} \cos(\frac{3\pi}{2}) = 0.$$

(b) As usual in order to find the standard deviations we need to calculate the uncertainty values for the position and momentum measurements according to the standard formula for $\hat{Q} = \hat{x}$ and $\hat{Q} = \hat{p}$ [109].

For this the evaluation of $\langle \hat{x}^2 \rangle_t$ and $\langle \hat{p}^2 \rangle_t$ is needed. Although it should be now straightforward it is maybe worth to point an alternative calculation for the average of the squared momentum, $\hat{p}^2$. This because for the infinite well, where $V(x) = 0$ we have,

$$\hat{H} = \frac{\hat{p}^2}{2m} \qquad \rightarrow \qquad \langle \hat{p}^2 \rangle_t = 2m \langle \hat{H} \rangle_t$$

This can be calculated very quickly by taking into account the eigenvalue equation for the eigenstates, and the orthnormalization condi-

108: Note that can also check that $\langle \hat{p} \rangle_t$ and $\langle \hat{x} \rangle_t$ via the Ehrefrenst commutation relations which in the present case takes the Newton's 2nd law form for the average values

$$\frac{d}{dt} \langle \hat{x} \rangle_t = \langle \hat{p} \rangle_t$$

109: Which is

$$\Delta \hat{Q}_t = \sqrt{\langle \hat{Q}^2 \rangle_t - \langle \hat{Q} \rangle_t^2}.$$

tions, $\hat{H}\phi_n = E_n\phi_n$. Then,

$$\begin{aligned}
\langle\hat{H}\rangle_t &= \langle\psi_t|\hat{H}|\psi_t\rangle = \frac{1}{2}\left(\langle\phi_1| + \imath e^{\imath\omega_0 t}\langle\phi_2|\right)|\hat{H}|\left(|\phi_1\rangle - \imath e^{-\imath\omega_0 t}|\phi_2\rangle\right) \\
&= \frac{1}{2}\left(|\langle\phi_1| + \imath e^{\imath\omega_0 t}\langle\phi_2|\right)\left(\hat{H}|\phi_1\rangle - \imath\hat{H}e^{-\imath\omega_0 t}|\phi_2\rangle\right) \\
&= \frac{1}{2}\left(|\langle\phi_1| + \imath e^{\imath\omega_0 t}\langle\phi_2|\right)\left(E_1|\phi_1\rangle - \imath E_2 e^{-\imath\omega_0 t}|\phi_2\rangle\right) \\
&= \frac{1}{2}(E_1\times(1) + E_2\times(1) + \imath E_1 e^{\imath\omega_0 t}\times(0) - \imath E_2 e^{-\imath\omega_0 t}\times(0)) \\
&= \frac{1}{2}(E_1 + 4E_1) = \frac{5}{2}E_1
\end{aligned}$$

Eventually we get,

$$\langle\hat{p}^2\rangle_t = 2m\langle\hat{H}\rangle_t = 5mE_1 = \frac{5\pi^2\hbar^2}{2L^2} = \text{const.} \tag{7.8}$$

Then the uncertainty is calculated as (with the use of (7.7)),

$$(\Delta\hat{p})_t = \sqrt{\langle\hat{p}^2\rangle_t - \langle\hat{p}\rangle_t^2} = \frac{\hbar}{L}\sqrt{\frac{5\pi^2}{2} - \frac{64}{9}\cos^2(\omega_0 t)}$$

Unfortunately no such trick is available for the calculation of $\langle x^2\rangle_t$ and one has to go through the algebraic manipulation.

CA2 Question 3 **(25 Marks)**

An electron is moving in the field of an HO potential with $\hbar\omega_0 = 0.04$ eV. Initially it is found in the excited state.

$$\psi(x,0) = \phi_4(x), \qquad n = 4, \text{ HO's eigenstate.}$$

(a) Provide the wavefunction $\phi_4(x)$ and a rough sketch for the probability distribution $|\phi_4(x)|^2$.

(b) What is the probability that the particle will be found in the classically allowed region?

(c) Find the particle's mean position and momentum values.

Solution The expression for the eigenstates/eigenenergies of the HO's Hamiltonian

$$\hat{H}_{ho} = \hat{p}^2/2m + m\omega_0^2\hat{x}^2/2$$

in the position-representation of a particle of mass m are as below,

$$\hat{H}_{ho}(x,p) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega_0^2x^2,$$

$$\hat{H}_{ho}\phi_n(x) = \phi_n(x), \qquad E_n = \hbar\omega_0(n+\frac{1}{2}), \quad n = 0,1,2,\cdots$$

$$\phi_n(x) = N_n e^{-\beta^2x^2/2}H_n(\beta x), N_n = \sqrt{\frac{\beta}{2^n n!\sqrt{\pi}}}$$

$$\beta = \sqrt{\frac{m\omega_0}{\hbar}}, \qquad H_n(x) \qquad \text{Hermite polynomials}$$

For this problem the (a) question is quite obvious how to go since is nothing else but the plot of the (known) eigenfunction of the HO, $\phi_4(x)$. Since

$$N_4 = \frac{1}{4}\sqrt{\frac{1}{6\sqrt{\pi}}}$$

$$\phi_4(x) = \frac{1}{4}\sqrt{\frac{1}{6\sqrt{\pi}}}\left(16(\beta x)^4 - 48(\beta x)^2 + 12\right)e^{-(\beta x)^2/2}$$

$$|\phi_4(x)|^2 = N_4^2 e^{-\beta^2x^2}H_4^2(\beta x)$$

(b) One needs to find the point x_4 where the particle cannot be found beyond this based on classical arguments. For ϕ_4 we have,

$$E_4 = \hbar\omega_0(4+\frac{1}{2}) = \frac{9}{2}\hbar\omega_0 = 0.18 \text{ eV}$$

Then, classical mechanics requires the velocities to be bound due to

the conservation of the total mechanical energy,

$$E_4 = \frac{1}{2}mv^2 + \frac{1}{2}m\omega_0^2 x^2 \qquad \rightarrow \qquad v = \sqrt{\frac{2}{m}(E_4 - \frac{1}{2}m\omega_0 x^2)}$$

Since $E_4 \geq \frac{1}{2}m\omega_0 x^2$ one can calculate that the classically allowed region is,

$$-x_4 \leq x \leq x_4, \qquad x_4 = \frac{2E_4}{m\omega_0^2} = \cdot$$

At this point we are ready to calculate the QM probability that a position measurement will find the particle within the classically allowed region,

$$P_4(-x_4 \leq x \leq x_4) = \int_{-x_4}^{x_4} dx|\phi_4(x)|^2 = \cdot \simeq 0.9210 \quad \text{check it!}$$

(**c**) Accordingly, the mean values for position and momentum can be found utilizing the QM formulas. But for these type of calculations a good number of examples are presented in the relevant chapter for HO.

CA2 Question 4 **(25 Marks)**

The Hamiltonian of a particle is given by [110] :

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega_0^2\hat{x}^2 - qE\hat{x}$$

(a) Derive the Ehrefenst equations of motions for the mean values of position, $\langle x\rangle_t$, and momentum, $\langle p\rangle_t$.

(b) Solve these equations when the above mean values are initially zero.

(c) Take the limit where $\omega_0 \to 0$ and give $\langle x\rangle_t$ and $\langle p\rangle_t$.

110: An example is an electron subject to an harmonic potential (e.g. quantum dot) placed in an electric field of magnitude E.

Solution **(a)** Here one can go and apply the Ehrefrenst theorem as demonstrated in the lectures and the notes. The difference is only in the extra term in the Hamiltonian ($-qE\hat{x}$). Here I provide only the final results for verification reasons of your own solutions:

$$\frac{d}{dt}\langle\hat{x}\rangle_t = \frac{\langle\hat{p}\rangle}{m}, \qquad \frac{d}{dt}\langle\hat{p}\rangle_t = -m\omega_0^2\langle\hat{x}\rangle + qE,$$

(b) The solution of the above equations proceeds now in the usual way where we take the time derivative of the first equation and substitute the second one,

$$\frac{d^2}{dt^2}\langle\hat{x}\rangle_t = \frac{1}{m}\frac{d}{dt}\langle\hat{p}\rangle = -\omega_0^2\langle\hat{x}\rangle_t + \frac{qE}{m}$$

Then we arrive at an driven HO problem for the mean-value of the position with a constant force:

$$\frac{d^2}{dt^2}\langle\hat{x}\rangle_t + \omega_0^2\langle\hat{x}\rangle_t = \frac{qE}{m}$$

subject to the initial conditions,

$$\langle\hat{x}\rangle_0 = 0, \qquad \langle\hat{p}\rangle_0 = 0.$$

The solution for this problem is,

$$\langle\hat{x}\rangle_t = \frac{qE}{m\omega_0^2}(1 - \cos\omega_0 t), \qquad \langle\hat{p}\rangle_t = \frac{qE}{\omega_0}\sin\omega_0 t,$$

(c) In order to take the limit $\omega_0 \to 0$ we have use the following approximations

$$\sin x \simeq x, \qquad \cos x \simeq 1 - \frac{x^2}{2}, \qquad x \to 0$$

Eventually we should arrive to

$$\langle\hat{x}\rangle_t \simeq \frac{qE}{2m\omega_0^2}t^2, \qquad \langle\hat{p}\rangle_t \simeq qEt,$$

which are the equations-of-motions if we had started with a free-particle (no motion in an HO potential $\omega_0 = 0$)) subject to an electric force $F = -qE$ only.