Quantum Mechanics II 2019

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These notes are not yet fully endorsed by myself and should be used with some caution. Note that lots of typos should be present. Also, please, do not hesitate to communicate such suspected typos or possible inaccuracies (Nov 2019)

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Chapter 1

Quantum mechanics formulation

Traditionally, the first encounter with QM theory and its applications is through the state vector formalism, may be just because it is the simpler choice (but not simple) conceptually; On a practical level, vastly, is the most economical one. The central concepts in this formulation for a physical system are (a) the physical states represented by the vector *state*, $|\psi\rangle$, (b) the observables $\mathcal{Q}$ represented by operators,$\hat{Q}$, and (c) the transformation rules when operators act on the vector states $\hat{Q}|\psi\rangle$), with the chief rule being the time-evolution laws, one deterministic (Schrödinger equation) and the other probabilistic (Measurement). All the predictions about a QM system are derived from these two central concepts, the abstract vector-states $|\psi\rangle$ and the observables-operators, $\hat{Q}$.

In the below, a set of QM axioms are listed, representing a merged version of the full set postulates stated in [**?**], where a more detailed discussion can be found.

States. The physical state of a system is represented by a vector ($|\psi\rangle$) belonging in some linear vector space $\mathcal{V}$.

Operators. A physical quantity ($\mathcal{Q}$) is represented by an operator ($\hat{Q}$). Their action on a vector state, $\hat{Q}|\psi\rangle$, is also a vector state of $\mathcal{V}$.

Time evolution. The time evolution of the vector state $|\psi\rangle$ is governed by the system's total energy operator, $\hat{H}$ as,

$$\imath\frac{d}{dt}|\psi\rangle = \hat{H}|\psi\rangle. \tag{1.1}$$

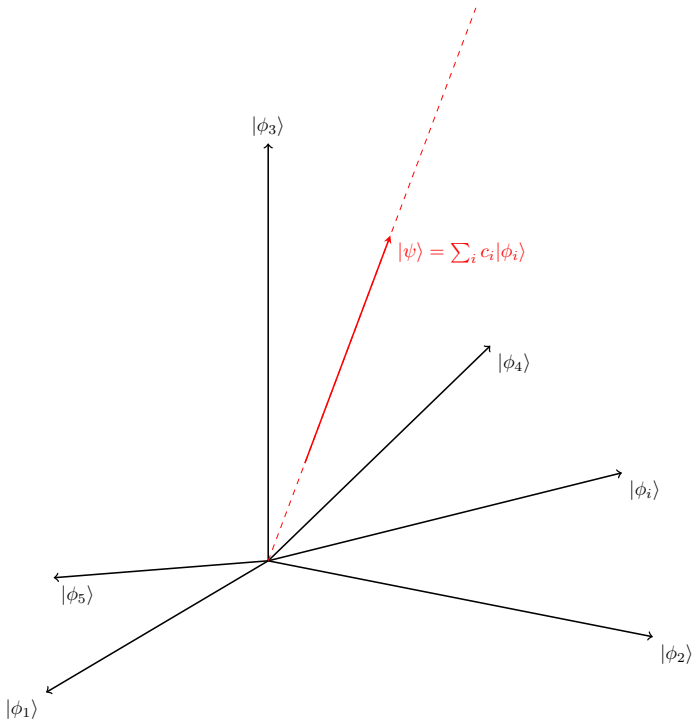


Figure 1.1: In quantum mechanics a physical state can be thought as a vector of the (abstract) Hilbert space spanned by the orthogonal eigenstates $|\phi_i\rangle$ of some observable operator, $\hat{Q}$. In accord to this geometrical picture any change of the state can be analyzed in terms of the observable's 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*.

Measurement. A measurement of $\mathcal{Q}$ changes the state $|\psi\rangle$ to an eigenstate $|q_n\rangle$ of $\hat{Q}$ with probability dependent on the eigenstate $|q_n\rangle$ and the state $|\psi\rangle$. The measurement returns the value q_n.

1.1 QM Vectors

Some additional notes are needed here. The abstract state $|\psi\rangle$ follows the Dirac convention and is also known as *ket* vector state. 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 $\mathcal{V}$.

The fact that the space $\mathcal{V}$ is a linear vector space has lots of important consequences with the most fundamental that *any linear combination of vector states belonging in $\mathcal{V}$ also belongs to $\mathcal{V}$, thus representing a physical state of the system.*

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

Moreover, as $\mathcal{V}$ is a linear vector space a complex-valued inner product between $|\chi\rangle$ and $|\phi\rangle$ is defined.This way one is ready to define the scalar inner product between two arbitrary states of $\mathcal{V}$ as the complex value, expressed as,

$$c(\chi, \phi) = \langle\chi|\phi\rangle$$

The practical consequences of the above abstract (and general) definitions become more evident when $\mathcal{F}$ is specialized.

A *complete* set of orthonormalised states $|\phi_n\rangle$ is defined when all $|\psi\rangle$ in $\mathcal{V}$ can be expressed in a unique way as,

$$|\psi\rangle = \sum_n c_n|\phi_n\rangle, \qquad c_n = \langle\phi_n|\psi\rangle \tag{1.2}$$

The above expansion is also known as *superposition expansion.* This set is named orthonormalized when $\langle\phi_n|\phi_m\rangle = \delta_{nm}$. In analogy with the childhood vector algebra learned in high-school the role of $|\psi_n\rangle$ is very similar with the Cartesian components of a the familial spatial vector [see Fig:(1.1)]; namely, if $\mathbf{A}$ is a vector in the 3D space, then its (Cartesian) coordinates (A_1, A_2, A_3) can be expressed along three - orthogonal directions $(\hat{x}_1, \hat{x}_2, \hat{x}_3)$ as,

$$\mathbf{A} = \sum_{i=1}^{3} A_i\hat{x}_i, \qquad A_i = \mathbf{A}\cdot\hat{x}_i, \qquad \hat{x}_i\cdot\hat{x}_j = \delta_{ij} \tag{1.3}$$

An additional formulation (meaning reexpressing the same thing) of (1.3) is obtained if we identify the 3-elements column basis, satisfying,

$$\hat{x}_1 \longrightarrow |x_1\rangle = \begin{pmatrix}1\\0\\0\end{pmatrix}, \qquad \hat{x}_1 \to |x_2\rangle = \begin{pmatrix}0\\1\\0\end{pmatrix}, \qquad \hat{x}_1 \longrightarrow |x_3\rangle = \begin{pmatrix}0\\0\\1\end{pmatrix} \tag{1.4}$$

$$\hat{x}_1^T \longrightarrow \langle x_1| = \big(1,0,0\big), \qquad \hat{x}_1^T \longrightarrow \langle x_2| = \big(0,1,0\big), \qquad \hat{x}_1^T \longrightarrow \langle x_3| = \big(0,0,1\big) \tag{1.5}$$

Given the above a physical 3D vector $\mathbf{A} = (A_1, A_2, A_3)$ with A_i real, $(A_i = A_i^*), i = 1, 2, 3$ may be expressed as,

$$\mathbf{A} \longrightarrow |A\rangle = A_1|x_1\rangle + A_2|x_2\rangle + A_3|x_3\rangle = \begin{pmatrix} A_1 \\ A_2 \\ A_3 \end{pmatrix}, \tag{1.6}$$

$$\mathbf{A}^T \longrightarrow \langle A| = A_1^*\langle x_1| + A_2^*\langle x_2| + A_3^*\langle x_3| = \left(A_1^*, A_2^*, A_3^*\right) \tag{1.7}$$

The generalization of the familiar 3D algebra is slightly more involved mainly for two reasons: (a) the dimensionality is higher (now it is not so easy to visualize a n-orthogonal vectors, $|\phi_n\rangle$, and (b) Inner product is complex valued, thus introducing the dual space basis vectors of $\mathcal{V}^\star$. For an $N-$dimensional state space,

$$|v_1\rangle = \begin{pmatrix} 1 \\ 0 \\ .. \\ 0 \end{pmatrix}, \qquad |v_2\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ .. \end{pmatrix}, ..., \quad |v_n\rangle = \begin{pmatrix} 0 \\ 0 \\ .. \\ 1 \\ .. \\ 0 \end{pmatrix}, \tag{1.8}$$

$$\langle v_1| = \left(1, .., 0\right), \qquad \langle v_2| = \left(0, 1, ..\right), ..., \quad \langle v_n| = \left(0, 0, .., 1, ..0\right), \tag{1.9}$$

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:

$$|\psi\rangle = \mathbf{C} = \begin{pmatrix} c_1 \\ c_2 \\ .. \\ c_n \\ .. \\ c_N \end{pmatrix} \qquad \langle\phi| = \mathbf{C}^T = \left(c_1^* ... c_N^*\right) \tag{1.10}$$

This way one can use matrix algebra to work out compactly and efficiently (suitable for numerical calculations) the (initially) abstract algebraic relations. For example, it is now immediately seen that the inner product of $|\psi\rangle$ with itself (multiplication of its bra with the ket state) is,

$$\langle\psi|\psi\rangle = \mathbf{C}^T \cdot \mathbf{C} = \left(c_1^*, ..., c_n^*, .., c_N^*\right) \begin{pmatrix} c_1 \\ ... \\ c_n \\ .. \\ c_N \end{pmatrix} = \sum_{n=1}^{N} |c_n|^2 \tag{1.11}$$

and that,

$$c_n = \langle \phi_n | \psi \rangle = \big(0, .., 1, ...0\big) \begin{pmatrix} c_1 \\ ... \\ c_n \\ .. \\ c_N \end{pmatrix} \tag{1.12}$$

Note that for normalized states the following is true:

$$\langle \psi | \psi \rangle = \sum_{n=1}^{N} |c_n|^2 = 1. \tag{1.13}$$

Quantum states should have finite magnitude ('length') if their projections to an arbitrary vector space are to intepreted as probability values.

1.2 QM Operators

Operators act on states. In QM operators are used to represent physical quantities, also known as *observables*. Examples are energy, position, translational and angular momentum, spin and generally any combination of them is also an observable. The mathematical expression of the observables arises quite easily when the corresponding classical operator exists e.g. position ($\mathbf{r}$), translational momentum ($\mathbf{p}$), by following the quantization rules, $\mathbf{x} \to \hat{x}$ and $\mathbf{p} \to -\imath\nabla$. If one thinks that most of the classical mechanics quantities can be expressed in terms of these two fundamental quantities (e.g. angular momentum, $\mathbf{L} = \mathbf{r} \times \mathbf{p}$) then this approach is sufficient. Not always though, as one can conclude from the case of the spin operator, a purely quantum operator with no classical counterpart.

In any case, when the observable is chosen, an associated operator exists which in turn defines a *complete set* of eigenvectors and eigenvalues as:

$$\hat{Q}|q_n\rangle = q_n|q_n\rangle, \qquad \langle q_n|q_m\rangle = \delta_{nm}, \qquad \sum_n |q_n\rangle\langle q_n| = \mathbb{1}, \tag{1.14}$$

where

$$\delta_{nm} = \begin{cases} 1 & n = m \\ 0 & n \neq m. \end{cases}$$

Noting that the eigenstate basis set of an observable (actually this is the requirement for a physical quantity to be an observable) is complete according to the superposition expansion (1.2) the ket state $|\psi\rangle$ can be expanded in terms of this eigenset:

$$|\psi\rangle = \sum_n c_n|q_n\rangle, \qquad c_n = \langle q_n|\psi\rangle. \tag{1.15}$$

Coefficient c_n has a very precise physical meaning upon a measurement of $\mathcal{Q}$. For now, it is needed to note that the observable $\mathcal{Q}$ is associated with the operator $\hat{Q}$ which acts in $|\psi\rangle$. However, for each $|\psi\rangle$ ket we have a $\langle\phi|$ bra and it is normal to wonder what kind of operator (associated with the observable $\mathcal{Q}$) acts to these states. It turns out that for an observable the conjugate (dual) operator acting in $\mathcal{V}^\star$ satisfies the conjugate eigenvalue equation[1] ,

$$\langle q_n|\hat{Q} = q_n\langle q_n|, \qquad \langle q_n|q_m\rangle = \delta_{nm}. \tag{1.16}$$

This means that for an arbitrary $|\psi\rangle$ ket or $\langle\phi|$ the action of an observable in the system if fully determined by the use of (1.15) and (1.14) and (1.16). For

[1]For an arbitrary operator (not necessarily an observable) if $\hat{A}|\psi_n\rangle = a_n|\psi_n\rangle$ then $\langle\psi_n|A^\dagger = a_n^\star\langle\psi_n|$.

example:

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

Vector spaces of finite dimension are named as Hilbert spaces. A further level of generalization arises when the basis is of infinite dimension. The complication is that that eigenvectors $|q_n\rangle$ are not normalized and vector spaces resulting from such bases via (1.15) should have inner products that result to probabilities lying necessarily between 0 and 1.

Algebraic (Matrix) representation of operators Along similar lines as for the algebraic representation of the $|\psi\rangle$ and $\langle\phi|$ as 1-dimensional matrices (rows and columns) we can extend this to two-index vectors, represented as matrices. If the fundamental basis is defined as $\hat{\mathcal{U}}_{ij} = |v_i\rangle\langle v_i|$ and its matrix representation as $\boldsymbol{\mathcal{U}}_{ij} = \mathbf{v}_i\mathbf{v}_j^T$,

$$\hat{\mathcal{U}}_{ij} = |v_i\rangle\langle v_j| \quad \leftrightarrow \quad \boldsymbol{\mathcal{U}}_{ij} = \mathbf{v}_i\mathbf{v}_j^T = \begin{bmatrix} 0 & 0 & 0 & 0 & ... & 0 \\ 0 & 0 & 0 & 0 & ... & 0 \\ ... & ... & \dots & ... & ... & 0 \\ 0 & 0 & \dots & 1 & ... & 0 \\ ... & ... & \dots & ... & ... & 0 \end{bmatrix} \tag{1.17}$$

then an arbitrary operator/matrix, $\hat{M}, \mathbf{M}$ can be expressed in the fundamental basis as,

$$\hat{M} = \sum_{ij} M_{ij}|v_i\rangle\langle v_j| = \sum_{ij} M_{ij}\hat{\mathcal{U}}_{ij} \tag{1.18}$$

$$\mathbf{M} = \sum_{ij} M_{ij}\boldsymbol{\mathcal{U}}_{ij} \tag{1.19}$$

It is straightforward to confirm that

$$M_{ij} = \langle v_i|\hat{M}|v_j\rangle \tag{1.20}$$

Representation of an observable on its own basis . From the above algeraic expressions for the matrix elements of an matrix is quite straightforward to show that the representation of an observable, $\hat{Q}$ on its eigenbasis $|q_n\rangle, n = 1, 2, ..$ is a diagonal matrix with entries its eigenvalues, properly ordered:

$$\hat{Q} = \sum_n q_n|q_n\rangle\langle q_n| = \begin{bmatrix} q_1 & 0 & 0 & 0 & ... & 0 \\ 0 & q_2 & 0 & 0 & ... & 0 \\ ... & ... & \dots & ... & ... & 0 \\ 0 & 0 & \dots & q_n & ... & 0 \\ ... & ... & \dots & ... & ... & 0 \end{bmatrix} \tag{1.21}$$

Projection Operator. An important mathematical object arises when one multiplies a ket of a state with its bra, namely, $P_\psi = |\psi\rangle\langle\phi|$,

$$\mathbf{P}_\psi = \mathbf{C}\cdot\mathbf{C}^T = \begin{pmatrix} c_1 \\ ... \\ c_n \\ .. \\ c_N \end{pmatrix} \left(c_1^*, ..., c_n^*, .., c_N^*\right) = \begin{bmatrix} |c_1|^2 & c_1c_2^* & \dots & c_1c_n^* & ... \\ c_2c_1^* & |c_2|^2 & \dots & c_2c_n^* & ... \\ ... & ... & \dots & ... & ... \\ c_nc_1^* & c_nc_2^* & \dots & |c_n|^2 & ... \\ ... & ... & \dots & ... & ... \end{bmatrix} \quad (1.22)$$

The above object, $\hat{P}_\psi$ is known as the projection operator of $|\psi\rangle$ for reasons that will be explained very soon. Obviously projection operator have the algebraic structure of a matrix but what it is more interesting about it is that it appears that it is an alternative construction to ket $|\psi\rangle$. In this particular case $|\psi\rangle$ and $\hat{P}_\psi$ are completely equivalent and one can use either the $|\psi\rangle$ or $\hat{P}_\psi$ to represent the state of the system. In such a context (where $\hat{P}_\psi$ is chosen to describe the state of the system) $\hat{P}_\psi$ is also known as density-operator state with $\mathbf{P}_\psi$ the corresponding density-matrix state representation expanded in an arbitrary basis. $|\psi\rangle$ is of course more economical, as the knowledge of N components are needed while for $\hat{P}_\psi$ one needs N^2 numbers for a complete determination[2]. Obviously, when it is not absolutely necessary the use of $|\psi\rangle$ is the preferential one.

With this notation the fundamental $\hat{P}_i$ projection operator is defined as

$$\hat{P}_i = |v_i\rangle\langle v_i|, \quad (1.23)$$

$$\hat{P}_i = \hat{P}_i^T, \qquad \hat{P}_i^2 = \hat{P}_i, \qquad \sum_i \hat{P}_i = \mathbb{1}. \quad (1.24)$$

where $\hat{P}_n$ is the basis projection matrix [see definition following (1.18),(1.19)].

[2]For normalized states since $\langle\psi|\psi\rangle = 1$ the number of unknowns is reduced by one

1.3 Probabilistic time evolution (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 leads to inconsistencies if pushed further, still a matter of debate, but it is not of concern here. Also, 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 [**?**] and references therein.

That said, let's now consider a system in a state $|\psi\rangle$ and an observable $\mathcal{Q}$. A measurement of $\mathcal{Q}$ will give the real eigenvalue q_n with probability, $P(q_n)$. If,

$$\hat{Q}_n = |q_n\rangle\langle q_n|$$

the appearance probability is equal to,

$$P(q_n) = \langle\psi|\hat{Q}_n|\psi\rangle = \langle\psi|\left(|q_n\rangle\langle q_n|\right)|\psi\rangle = \langle q_n|\psi\rangle^{\star}\langle q_n|\psi\rangle = |\langle q_n|\psi\rangle|^2 \quad (1.25)$$

The state of the system immediately afterwards is proportional to $|q_n\rangle$. Accordingly, the matrix representation of the operator $\hat{Q}_n$ is given by:

$$(Q_n)_{ij} = \langle v_i|\hat{Q}_n|v_j\rangle \quad (1.26)$$

The measurement process can be put on a more formal basis as follows[3]:

Measurement of $\mathcal{Q}$ in state $|\psi\rangle$ gives the value q_n with probability $P(q_n)$ and leaves the system in state

$$P(q_n) = \langle\psi|\hat{Q}_n|\psi\rangle \quad \rightarrow \quad |\psi_n\rangle = \frac{\hat{Q}_n|\psi\rangle}{\sqrt{\langle\psi|\hat{Q}_n|\psi\rangle}}, \quad (1.27)$$

[3]The below definition is suitable both for generate and non-degenerate eigenvalue spectrum, provided a proper definition of the projection operator, $\hat{Q}_n$, is introduced.

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[4], the choice of a particular coordinate system, say $\mathcal{C}$ 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 ($\mathcal{C} \rightarrow \mathcal{C}'$) transforms the original set of component, expressed in $\mathcal{C}$), in a controlled way, to another set of components (expressed now in $\mathcal{C}'$)[5]. 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 in the spherical and orthogonal coordinate systems. What would be the wiser choice? 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 is that quantum physical states (and operators) live in linear vector spaces and dealing with quantum mechanical systems more often than not a suitable complete basis set must be chosen. The abstract quantum basis set used to expand the abstract vectors corresponds to the (spatial) coordinate system of classical mechanics. Also, often the basis is dictated by the observable ($\mathcal{Q}$) under question and the type of the measurement to be performed and not only the system itself. Fortunately, the operator associated with the observable offer through its eigenvalue equation a recipe to generate a complete basis set. Picking the right observable and solving the eigenvalue equation is a step that one needs to go through in most cases.

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

[5]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 ($\mathcal{C}$) or $\mathcal{C}'$

Normalization and energy measurements of a state $|\psi_0\rangle$

Assume a quantum system with three possible states with two of them doubly degenerate ($\omega_0 = \epsilon_1 < \epsilon_2 = \epsilon_3 = 2\omega_0$), initially in the normalized (coherent) superposition,

$$|\psi_0\rangle = \sum_{n=1}^{3} c_n|\phi_n\rangle = c_1|\phi_1\rangle + \frac{1}{2}|\phi_2\rangle + \frac{1}{2}|\phi_3\rangle, \tag{1.28}$$

Let's set $\epsilon_1 = \hbar\omega_0$ and $\epsilon_2 = \epsilon_3 = 2\hbar\omega_0$. Next we consider the energy observable $\mathcal{H}$.
(a) Assume that the energy measurement takes place at time $t_0 = 0$. What results one should expect and how probable they are.
(b) What are the expectation values for the energy and its standard deviation?
(c) Assume that we had let first the system evolve for time t and then to perform the energy measurements. What the results of (b) question would then be?
(a)
The operator of the energy observable $\mathcal{H}$ is (of course) the Hamiltonian operator, $\hat{H}$ and the following QM postulates hold,

$$\hat{H}|\phi_n\rangle = \epsilon_n|\phi_n\rangle, \qquad n, m = 1 - 3 \tag{1.29}$$

$$\langle\phi_n|\phi_m\rangle = \delta_{nm}, \qquad \sum_{n=1}^{3} |\phi_n\rangle\langle\phi_n| = \mathbb{1}. \tag{1.30}$$

Normalization. First things first, is to normalize the state at the time of observation, which, of course is given by (1.28). 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. Despite the fact that is unknown[a] a good amount of information can still be extracted. So the initial state is,

$$|\psi_0\rangle = \frac{e^{\imath\theta}}{\sqrt{2}}|\phi_1\rangle + \frac{1}{2}|\phi_2\rangle + \frac{1}{2}|\phi_3\rangle. \tag{1.31}$$

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

$$|\psi\rangle = \sum_n c_n|q_n\rangle, \qquad c_n = \langle q_n|\psi\rangle.$$

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

$$P(E = \epsilon_n) = |\langle\phi_n|\psi_0\rangle|^2 = |c_n|^2.$$

[b] 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:

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

[a] Note that the (relative) phase of a quantum state in linear superposition matters (in contrast with a global phase e.g. $e^{\imath\phi}|\psi_0\rangle$).

[b] These probabilities can also be found from the generalized definition of the projection operator, $\hat{Q}_n = |\phi_n\rangle\langle\phi_n| \longrightarrow P(q_n) = \langle\psi|\hat{Q}_n|\psi\rangle = \langle\psi|(|\phi_n\rangle\langle\phi_n|)|\psi\rangle = \langle\psi|\phi_n\rangle\langle\phi_n|\psi\rangle|\langle\psi|\phi_n\rangle|^2$.

Energy mean value and standard deviation of a state $|\psi_0\rangle$

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, $\hat{Q}$

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

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

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

where the orthonormalization condition were used for the calculation of the inner products $\langle\phi_n|\phi_m\rangle$ according the orthonormality rules of (1.30),

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

An alternative method. An alternative, fast track, calculation of the mean energy value can be obtained by relying in matrix operations if we decide to represent operators and vectors on the (fundamental) vector basis (1.8)]. Then,

$$\hat{H} = \hbar\omega_0\begin{pmatrix}1&0&0\\0&2&0\\0&0&2\end{pmatrix}, \qquad |\psi\rangle = \frac{1}{2}\begin{pmatrix}e^{\imath\theta}\sqrt{2}\\1\\1\end{pmatrix} \tag{1.32}$$

We then immediately get,

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

Standard deviation of a state $|\psi_0\rangle$

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

$$\Delta Q_\psi = \sqrt{\langle\psi|(\hat{Q}-\langle Q\rangle_\psi)^2|\psi\rangle} = \sqrt{\langle \mathcal{Q}^2\rangle_\psi - \langle\mathcal{Q}\rangle_\psi^2} \neq 0. \tag{1.33}$$

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, $\hat{Q}$

$$\Delta H_\psi = \sqrt{\langle\psi|(\hat{H}-\langle H\rangle_\psi)^2|\psi\rangle} = \sqrt{\langle \hat{H}^2\rangle_\psi - \langle\hat{H}\rangle_\psi^2}. \tag{1.34}$$

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

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

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 (1.30),

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

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 (1.8)]. Then,

$$\hat{H}^2 = \hbar\omega_0\begin{pmatrix}1&0&0\\0&2&0\\0&0&2\end{pmatrix}\hbar\omega_0\begin{pmatrix}1&0&0\\0&2&0\\0&0&2\end{pmatrix} = (\hbar\omega_0)^2\begin{pmatrix}1&0&0\\0&4&0\\0&0&4\end{pmatrix}, \qquad |\psi\rangle = \frac{1}{2}\begin{pmatrix}e^{\imath\theta}\sqrt{2}\\1\\1\end{pmatrix} \tag{1.35}$$

We then immediately get,

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

Finally the standard deviation is

$$\Delta H_0 = \sqrt{\langle\hat{H}^2\rangle_0 - \langle\hat{H}\rangle_0^2} = \sqrt{\frac{5}{2}(\hbar\omega_0)^2 - \frac{9}{4}(\hbar\omega_0)^2} = \frac{1}{2}\hbar\omega_0 \tag{1.36}$$

Question: Energy mean value and standard deviation of a state $|\psi(t)\rangle$?

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,

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

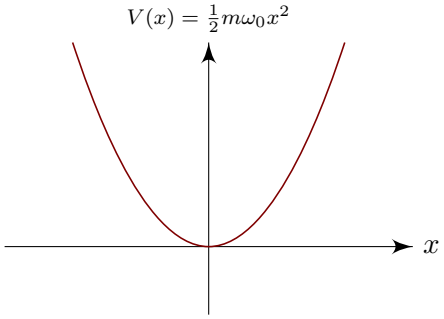
Since the $c_n(0)$ are known and $n = 1 - 3$ we end up to the following expression for the state of the current system:

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

You may try to repeat the calculations as in the case of $|\psi_0\rangle$.

Chapter 2

The quantum 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 equillibrium position (assumed to be at $x = 0$) is $V(x) = m\omega_0 x^2/2$.

EOM for classical HO

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,

$$E = E = \frac{1}{2}mv^2 + \frac{1}{2}m\omega_0^2 x^2 = \frac{p^2}{2m} + \frac{1}{2}m\omega_0^2 x^2 = \text{cnst} = \frac{1}{2}m\omega_0^2 A_0^2 \quad (2.1)$$

2.1 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 (2.1). 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,

$$\hat{H}_{ho} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega_0^2\hat{x}^2. \tag{2.2}$$

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:

$$\hat{x} = x \qquad \hat{p} = -\imath\hbar\frac{d}{dx}. \tag{2.3}$$

By replacing expressions (2.3) into (2.2) we obtain:

$$H_{ho} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega_0^2x^2 \tag{2.4}$$

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, [1] [1] where, $\psi(x,t) = \langle x|\psi(t)\rangle$

$$\imath\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}_{ho}|\psi(t)\rangle \qquad \longrightarrow \qquad \imath\frac{\partial}{\partial t}\psi(x,t) = \hat{H}_{ho}\psi(x,t) \tag{2.5}$$

2.2 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 [2] and bounded from below. So, we have, [3]

$$\hat{H}_{ho}|\phi_n\rangle = E|\phi_n\rangle \qquad \Longrightarrow \qquad \hat{H}_{ho}\phi_n(x) = E\phi_n(x)$$

Substituting the HO hamiltonian (2.4) gives,

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega_0^2 x^2\right)\phi_n(x) = E_n\phi_n(x) \tag{2.6}$$

Defining,

$$\beta \equiv \sqrt{\frac{m\omega_0}{\hbar}} \tag{2.7}$$

the HO eigenfunctions and the corresponding eigenenergies are expressed as, [4]

Harmonic oscillator spectrum

$$\phi_n(x) = N_n H_n(\beta x)e^{-\frac{1}{2}\beta^2 x^2}, \qquad E_n = \hbar\omega\left(n+\frac{1}{2}\right), \qquad n = 0, 1, 2, \cdots \tag{2.8}$$

$$\beta = \left(\frac{m\omega}{\hbar}\right)^{\frac{1}{2}}, \qquad N_n = \sqrt{\frac{\beta}{2^n n!\sqrt{\pi}}}$$

The QM orthonormalization and completeness relations for the $|\phi_n\rangle$,

$$\langle\phi_n|\phi_m\rangle = \delta_{nm} \qquad \mathbb{1} = \sum_n |\phi_n\rangle\langle\phi_n| \tag{2.9}$$

in the position representation the orthogonality condition become [5],

$$\langle\phi_n|\phi_m\rangle = \int_{-\infty}^{\infty} dx\, \phi_n^*(x)\phi_m(x) = \delta_{nm} = \begin{cases} 1 & n = m \\ 0 & n \neq m. \end{cases} \tag{2.10}$$

$$\sum_n \phi_n(x)\phi(x') = \delta(x - x') \tag{2.11}$$

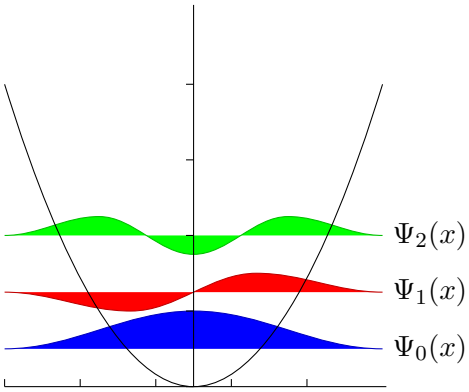
We also see that any physical state (say $|\psi\rangle$) of the particle in the HO potential can be expressed in terms of the HO eigenstates. This can be seen by taking the

[2] *Spectrum* in this context is used to describe the set of the eigenstates/eigenergies of an observable. The detailed derivation is given in section (2.5

[3] where, as usual

$$\phi_n(x) = \langle x|\phi_n\rangle$$
$$\hat{H}_{ho}\phi_n(x) = \langle x|\hat{H}_{ho}|\phi_n\rangle$$

[4]).



[5] To this the following properties of the position-eigenstates were used:

$$\int dx|x\rangle\langle x| = \mathbb{1}$$
$$\langle x|x'\rangle = \delta(x - x').$$

completeness relation and by multiplying from the left to obtain,

$$|\psi\rangle = \sum_n |\phi_n\rangle\langle\phi_n|\psi\rangle = \sum_n c_n|\phi_n\rangle, \qquad c_n = \langle\phi_n|\psi\rangle \tag{2.12}$$

Now by assuming the position-representation, we can multiple again from the left with $\langle x|$ to obtain:

$$\psi(x) = \sum_n c_n\phi_n(x), \qquad c_n = \int_{-\infty}^{\infty} dx\, \phi_n^*(x)\psi(x), \tag{2.13}$$

where $\psi(x) = \langle x|\psi\rangle$ and $\phi_n = \langle x|\phi_n\rangle$.

2.3 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:

$$\hat{Q}|\phi_n\rangle = q_n|\phi_n\rangle \qquad \Longrightarrow \qquad \hat{Q}\phi_n(x) = q_n\phi_n(x)$$

[6]

(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.)

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:

$$P(E = E_n, t) = |c_n(t)|^2 = |c_n e^{-\imath\omega_0(n+1/2)}| = |c_n|^2. \qquad \textbf{(constant in time)}$$

[6] Where Q is the representation of $\hat{Q}$ in the x-representation. One example of such operator is,

$$\hat{a} = \frac{1}{\sqrt{2}}(x + \hat{p}) = \frac{1}{\sqrt{2}}(x - \imath\hbar\frac{d}{dx}).$$

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.

$$\psi(t) = \frac{1}{\sqrt{6}}(\phi_0 e^{-\imath\omega_0 t/2} + 2\phi_1 e^{-3\imath\omega_0 t/2} + i\phi_4 e^{-9\imath\omega_0 t/2}).$$

2.4 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.[7]

2.4.1 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:

$$|\psi\rangle = \sum_n c_n(0)|\phi_n\rangle \qquad \rightarrow \qquad |\psi(t)\rangle = \sum_n c_n(0)e^{-\imath E_n t/\hbar}|\phi_n\rangle \tag{2.14}$$

In the position representation by recalling (2.15) one has,

$$\psi(x,0) = \sum_n c_n\phi_n(x) \qquad \Longrightarrow \qquad \psi(x,t) = \sum_n c_n e^{-\imath\omega_0(n+1/2)}\phi_n(x). \tag{2.15}$$

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):

$$\langle\hat{Q}(t)\rangle_\psi = \langle\psi(t)|\hat{Q}|\psi(t)\rangle = \sum_{nm} c_n^*(0)c_m(0)e^{\imath(E_n-E_m)t/\hbar}Q_{nm}, \tag{2.16}$$

$$Q_{nm} = \langle\phi_n|\hat{Q}|\phi_m\rangle. \tag{2.17}$$

In the case of the HO (and again within the chosen position representation) the QM expression for mean values of observables (2.16) specializes to,

$$\langle\hat{Q}\rangle(t) = \langle\psi(t)|\hat{Q}|\psi(t)\rangle = \sum_{nm} c_n^*c_m e^{\imath\omega_0(n-m)t}Q_{nm}, \tag{2.18}$$

$$Q_{nm} = \int_{-\infty}^{\infty} dx\, \phi_n^*(x)\hat{Q}\phi_m(x) \tag{2.19}$$

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: [8]

$$H_{nm} = E_m\int_{-\infty}^{\infty} dx\, \phi_n^*(x)\phi_m(x) = E_m\delta_{nm} \qquad \rightarrow \qquad \langle H(t)\rangle = \sum_n E_n|c_n|^2$$

[7] 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

[8] 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 (2.18) and (2.19) 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 $\langle\hat{p}\rangle$ [9].

[9] 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)

$$x_{nm} = \langle\phi_n|\hat{x}|\phi_m\rangle = \int_{-\infty}^{\infty} dx\, \phi_n^*(x) x \phi_m(x) \tag{2.20}$$

(ii)

$$p_{nm} = \langle\phi_n|\hat{p}|\phi_m\rangle = \int_{-\infty}^{\infty} dx\, \phi_n^*(x)) \left(-\imath\frac{d}{dx}\right) \mathbf{1}\phi_m(x) \tag{2.21}$$

Example: Mean value, standard deviation of $\hat{x}$ in state $|\phi_n\rangle$

$$\begin{aligned}
\langle x\rangle_n = x_{nn} &= \int_{-\infty}^{\infty} dx\, \phi_n^*(x) x \phi_n(x) = \int_{-\infty}^{\infty} dx\, N_n e^{-\beta^2 x^2/2} H_n(\beta x) x N_n e^{-\beta^2 x^2/2} H_n(\beta x) = N_n^2 \int_{-\infty}^{\infty} dx\, x e^{-\beta^2 x^2} H_n^2(\beta x) \\
&= \frac{N_n^2}{\beta^2}\left[\int_{-\infty}^{0} d(\beta x)\,(\beta x) e^{-(\beta x)^2} H_n^2(\beta x) + \int_0^{\infty} d(\beta x)\,(\beta x) e^{-(\beta x)^2} H_n^2(\beta x)\right] \\
&= \frac{N_n^2}{\beta^2}\left[\int_{-\infty}^{0} d(-\beta x)\,(-\beta x) e^{-(-\beta x)^2} [(-1)^n H_n(-\beta x)]^2 + \int_0^{\infty} d(\beta x)\,(\beta x) e^{-(\beta x^2)} H_n^2(\beta x)\right] \\
&= \frac{N_n^2}{\beta^2}\left[\int_{-\infty}^{0} du\, u e^{-u^2} H_n^2(u) + \int_0^{\infty} dv\, v e^{-v^2} H_n^2(v)\right] = \frac{N_n^2}{\beta^2}\left[-\int_{\infty}^{0} du\, u e^{-u^2} H_n^2(u) + \int_0^{\infty} dv\, v e^{-v^2} H_n^2(v)\right] = 0
\end{aligned}$$

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,

$$\begin{aligned}
\langle x^2\rangle_n = x_{nn}^2 &= \int_{-\infty}^{\infty} dx\, \phi_n^*(x) x^2 \phi_n(x) = N_n^2 \int_{-\infty}^{\infty} dx\, x e^{-\beta^2 x^2} H_n^2(\beta x) = \frac{N_n^2}{\beta^2}\int_{-\infty}^{+\infty} dx\, e^{-\beta^2 x^2}\,(\beta x H_n(\beta x))^2 \\
&= \frac{N_n^2}{\beta^2}\int_{-\infty}^{+\infty} dx\, e^{-\beta x^2}\left(\frac{1}{2}H_{n+1}^2(\beta x) + n H_{n-1}(\beta x)\right)^2 = \frac{N_n^2}{\beta^2}\int_{-\infty}^{+\infty} dx\, e^{-\beta x^2}\left[\frac{1}{4}H_{n+1}^2(\beta x) + n^2 H_{n-1}^2(\beta x) + n H_{n+1}(\beta x) H_{n-1}(\beta x)\right] \\
&= \frac{N_n^2}{\beta^2}\int_{-\infty}^{+\infty} dx\, e^{-\beta^2 x^2}\left[\frac{1}{4N_{n+1}^2} N_{n+1}^2 H_{n+1}^2(\beta x) + \frac{n^2}{N_{n-1}^2} N_{n-1}^2 H_{n-1}^2(\beta x) + \frac{n}{N_{n+1}N_{n-1}} N_{n+1} H_{n+1}(\beta x) N_{n-1} H_{n-1}(\beta x)\right] \\
&= \frac{1}{\beta^2}\left[(\frac{N_n}{2N_{n+1}})^2 \cancelto{1}{\langle\phi_{n+1}|\phi_{n+1}\rangle} + (\frac{nN_n}{N_{n-1}})^2 \cancelto{1}{\langle\phi_{n-1}|\phi_{n-1}\rangle} + \frac{nN_n}{N_{n+1}N_{n-1}} \cancelto{0}{\langle\phi_{n+1}|\phi_{n-1}\rangle}\right] = \frac{1}{\beta^2}\left[(\frac{N_n}{2N_{n+1}})^2 + (\frac{nN_n}{N_{n-1}})^2\right] \\
&= \frac{1}{\beta^2}\left[\frac{n+1}{2} + \frac{n}{2}\right] = \frac{1}{\beta^2}(n+\frac{1}{2}) = \frac{\hbar}{m\omega_0}(n+\frac{1}{2}) = \frac{E_n}{m\omega_0^2}.
\end{aligned}$$

To perform the above integrals the following relations were used,

$$x H_n(x) = H_{n+1}(x) + n H_{n-1}(x), \qquad \langle\phi_n|\phi_m\rangle = \delta_{nm}, \qquad N_n = \sqrt{\frac{\beta}{2^n n!\sqrt{\pi}}}$$

Finally we end up to following general properties for an HO in its eigenstate:

$$\langle x\rangle_n = 0, \qquad \langle x^2\rangle_n = \frac{E_n}{m\omega_0^2} \qquad \Delta x_n = \sqrt{\frac{E_n}{m\omega_0^2}} \tag{2.22}$$

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,

$$\begin{aligned}
\langle p\rangle_n = \hat{p}_{nn} &= \int_{-\infty}^{\infty} dx\, \phi_n^*(x)\hat{p}\phi_n(x) = N_n^2 \int_{-\infty}^{\infty} dx\, e^{-\beta^2x^2/2} H_n(\beta x)(-\imath\hbar\frac{d}{dx})\left[e^{-\beta^2x^2/2}H_n(\beta x)\right] \\
&= N_n^2 \int_{-\infty}^{\infty} dx\, e^{-\beta^2x^2/2} H_n(\beta x)\left[\imath\hbar x\beta^2 e^{-\beta^2x^2/2}H_n(\beta x) - \imath\hbar\beta e^{-\beta^2x^2/2}\frac{d}{d(\beta x)}H_n(\beta x)\right] \\
&= \imath\hbar \int_{-\infty}^{\infty} dx\, x N_n^2\beta^2 e^{-\beta^2x^2} H_n^2(\beta x) - \imath\hbar\beta \int_{-\infty}^{\infty} dx\, N_n e^{-\beta^2x^2/2} H_n(\beta x) e^{-\beta^2x^2/2}\left[2nH_{n-1}(\beta x)\right] \\
&= \imath\hbar \cancelto{0}{\langle\phi_n|x|\phi_n\rangle} - 2\imath\hbar\beta\frac{2n}{N_{n-1}}\int_{-\infty}^{\infty} dx\, \left(N_n e^{-\beta^2x^2/2}H_n(\beta x)\right)\left(N_{n-1}e^{-\beta^2x^2/2}H_{n-1}(\beta x)\right) \\
&= -2\imath\hbar\beta\frac{2n}{N_{n-1}}\cancelto{0}{\langle\phi_n|\phi_{n-1}\rangle} = 0
\end{aligned}$$

To perform the above integrals the following relations were used,

$$\frac{d}{dx}H_n(\beta x) = \beta\frac{d}{d(\beta x}H_n(\beta x) = \beta H'(u) = \beta 2nH_{n-1}(u) = 2n\beta H_{n-1}(\beta x) \qquad \rightarrow \qquad \frac{d}{dx}H_n(\beta x) = 2n\beta H_{n-1}(\beta x) \qquad \langle\phi_n|\phi_{n-1}\rangle = 0,$$

The standard deviation of the mean value is now given by,

$$\Delta p_n = \sqrt{\langle\hat{p}^2\rangle_n - \cancelto{0}{\langle\hat{p}\rangle_n}} \qquad \rightarrow \qquad \Delta p_n = \sqrt{\langle\hat{p}^2\rangle_n}$$

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 (2.2) we have,

$$\langle\hat{p}^2\rangle = 2m\langle\hat{H}\rangle - m^2\omega_0^2\langle x^2\rangle = 2mE_n - m^2\omega_0^2\frac{E_n}{m\omega_0^2} = mE_n, \tag{2.23}$$

where the mean value of $\langle\hat{x}^2\rangle$ used from (2.24) and that $\langle H\rangle = E_n$.

Finally we end up to following general properties for an HO in its eigenstate:

$$\langle p\rangle_n = 0, \qquad \langle p^2\rangle = mE_n, \qquad \Delta p_n = mE_n = \sqrt{mE_n}, \tag{2.24}$$

Based on the above results we can also evaluate the Heisenberg's relation for an HO in the state $|\phi_n\rangle$:

$$\Delta x_n\Delta p_n = \sqrt{\frac{E_n}{m\omega_0^2}}\sqrt{mE_n} = \frac{E_n}{\omega_0} = \hbar(n+\frac{1}{2}). \tag{2.25}$$

[10] [10] Therefore the uncertainty relation takes its minimum value when the system is in its ground state ($\phi_0(x)$):

$$\Delta x_0\Delta p_0 = \frac{\hbar}{2}$$

2.4.2 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 [11] . Examples of such observables are the usual operators such as the position, momentum, energy, etc.. Then we have,

$$\imath\hbar \frac{d}{dt}\langle \hat{Q} \rangle = \langle [\hat{Q},\ \hat{H}_{ho}] \rangle \frac{1}{2m} \langle [\hat{Q},\ \hat{p}^2] \rangle + \frac{1}{2} m\omega_0^2 \langle [\hat{Q},\ \hat{x}^2] \rangle.$$

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

$$\begin{aligned} [\hat{x},\ \hat{x}^2] &= [\hat{p},\ \hat{p}^2] = 0, \\ [\hat{x},\ \hat{p}^2] &= 2\imath\hbar\hat{p}, \\ [\hat{p},\ \hat{x}^2] &= -2\imath\hbar\hat{x}, \end{aligned}$$

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, [12]

$$\begin{aligned} \frac{d}{dt}\langle \hat{x} \rangle &= \frac{\langle \hat{p} \rangle}{m} \\ \frac{d}{dt}\langle \hat{p} \rangle &= -m\omega_0^2 \langle \hat{x} \rangle \end{aligned}$$

So given the mean values of the system's momentum and position at some time (say $t_0 = 0$) the corresponding solutions are,

[11] So $\frac{\partial \hat{Q}}{\partial t} = 0$.

[12] The first equation resembles the classical definition of momentum while the second one the equation of motion for the classical simple HO (after replacing $\frac{d}{dt}\langle \hat{x} \rangle = \langle \hat{p} \rangle$) :

$$\frac{d^2}{dt^2}\langle \hat{x} \rangle + \omega_0^2 \langle \hat{x} \rangle = 0.$$

$$\langle x\rangle(t) = x_0 \cos\omega_0 t + \frac{p_0}{m\omega_0}\cos\omega_0 t, \qquad x_0 = \langle x\rangle(0) \tag{2.26}$$

$$\langle p\rangle(t) = p_0 \cos\omega_0 t - m\omega_0 x_0 \sin\omega_0 t, \qquad p_0 = \langle p\rangle(0) \tag{2.27}$$

Therefore the classical equations of motion are still valid in the quantum case, however for the corresponding expectation values! [13]

[13] 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!

2.5 Solution of the HO eigenvalue equation*

[14] The objective in this section is to provide the solution procedure for the HO's eigenvalue equation (). We have,

[14] ***Not necessary for the final exams**

$$\begin{aligned}
&\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{1}{2}m\omega_0^2x^2\right)\phi(x)=E\phi(x),\\
\rightarrow\quad &\frac{d^2\phi(x)}{dx^2}-\left[(\frac{m\omega_0}{\hbar})^2\,x^2-\frac{2mE}{\hbar^2}\right]\phi(x)=0,\\
\rightarrow\quad &\frac{d^2\phi(x)}{dx^2}-\frac{m\omega_0}{\hbar}\left[\frac{m\omega_0}{\hbar}\,x^2-\frac{2E}{\hbar\omega_0}\right]\phi(x)=0\\
\rightarrow\quad &\frac{d^2\phi(x)}{d(\beta x)^2}-\left[(\beta x)^2-\frac{2E}{\hbar\omega_0}\right]\phi(x)=0,
\end{aligned}$$

where the β parameter (2.7) was introduced [15]. At this stage is convenient to introduce the scaled variables, X and $\mathcal{E}$ we end up to,

[15]
$$\beta=\sqrt{\frac{m\omega_0}{\hbar}}$$

$$X=\left(\frac{m\omega_0}{\hbar}\right)^{\frac{1}{2}}x=\beta x,\qquad \mathcal{E}=\frac{E}{\hbar\omega},\tag{2.28}$$

both of which is dimensionless. Then we are left with

$$\phi''(X)-(X^2-2\mathcal{E})\phi(X)=0,\tag{2.29}$$

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 [16],

$$\Phi(X)=h(X)e^{-\frac{1}{2}X^2}.\tag{2.30}$$

Then the Schrödinger equation gives,

$$\boxed{h''(X)-2Xh'(X)+(2\mathcal{E}-1)=0.}\tag{2.31}$$

This is known as *Hermite's equation* a well-studied differential equation in the 19th century [17]

[16] The rationale for this change goes as follows: For large X, such that $X^2\gg\mathcal{E}$ the term $\mathcal{E}\phi(X)$ cannot offset $X^2\phi(X)\to\infty$. 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 $\sim -X^2e^{-X^2}$.

[17] 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.

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,

$$\sum_{r\geq 0}\left[(r+2)(r+1)c_{r+2}+(2\mathcal{E}-1-2r)c_r\right]X^r=0.$$

In order the above to be true for all powers it is required that,

$$\frac{c_{r+2}}{c_r}=\frac{2r+1-2\mathcal{E}}{(r+2)(r+1)}\qquad r\geq 0.$$

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

$$2n+1-2\mathcal{E}=0\qquad\rightarrow\qquad\mathcal{E}_n=n+\frac{1}{2}\qquad\rightarrow\qquad\boxed{E_n=\hbar\omega_0(n+\frac{1}{2}),\quad n=0,1,2,..}$$

The latter relation gives the (now) quantized energies, E_n. For any given $n=0,1,2..$ the expansion solution is now given by, [18]

$$H_n(X)=\sum_r^n 2c_r\frac{r-n}{(r+2)(r+1)}X^r,\qquad r=\begin{cases}0,2,\cdots,n & \text{n even}\\ 1,3,\cdots,n & \text{n odd}\end{cases}\tag{2.32}$$

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

$$\begin{aligned}H_0(X)&=c_0\\ H_1(X)&=c_1X\\ H_2(X)&=c_0(1-2X^2)\\ H_3(X)&=c_1\left(X-\frac{2}{3}X^3\right).\end{aligned}$$

These are known as the *Hermite polynomials*. [19] By combining (2.30) and (2.32) we obtain the HO eigenfunctions as ,

$$\phi_n(x)=N_nH_n(\beta x)e^{-\beta^2x^2/2}\tag{2.33}$$

with a slight change of notation ($\Phi_n(X)=\Phi_n(\beta x)=\phi_n(x)$).

[18] Note the change of notation $h(X)\rightarrow H_n(X)$ to emphasize that one is restricted to Hermite polynomials H_n.

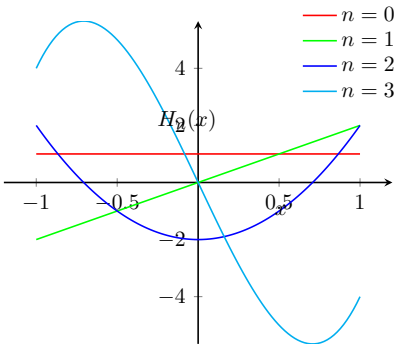


Figure 2.1: The graph of some Hermite polynomials.

[19] 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:

$$\begin{aligned}H_0(x)&=1,\qquad H_1(x)=2x\\ H_2(x)&=4x^2-2,\quad H_3(x)=8x^3-12x\\ \delta_{nm}(2^nn!\sqrt{\pi})&=\int_{-\infty}^{\infty}dx\,e^{-x^2}H_n(x)H_m(x)\\ H_n(-x)&=(-1)^nH_n(x)\\ H_n'(x)&=2nH_{n-1}(x),\\ H_{n+1}(x)&=2xH_n(x)-2nH_{n-1}(x)\\ H_{n+1}(x)&=2xH_n(x)-H_n'(x)\end{aligned}$$

2.6 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:

$$\langle T\rangle_t = \frac{n}{2}\langle V\rangle_t, \qquad V(x) = ax^n. \tag{2.34}$$

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,

$$\langle T\rangle_n = \langle V\rangle_n = \frac{E_n}{2} \tag{2.35}$$

(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: [20]

(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.)

[20] 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,

$$\hat{x}\phi_n(x) = \sqrt{\frac{\hbar}{2m\omega_0}}\left[\sqrt{n+1}\phi_n(x) + \sqrt{n}\phi_{n-1}(x)\right] \tag{2.36}$$

(b) Using the above calculate the arbitrary (dipole) matrix elements:

$$x_{nn'} = \langle\phi_n|\hat{x}|\phi_{n'}\rangle = ? \tag{2.37}$$

(4) **Matrix elements of** op**, $p_{nn'}$.**

(a) Use the properties of the Hermite polynomials to show that,

$$\hat{p}\phi_n(x) = \sqrt{\frac{m\omega_0}{2\hbar}}\left[\sqrt{n+1}\phi_n(x) - \sqrt{n}\phi_{n-1}(x)\right] \tag{2.38}$$

(b) Using the above calculate the arbitrary (dipole) matrix elements:

$$p_{nn'} = \langle \phi_n | \hat{p} | \phi_{n'} \rangle = ? \tag{2.39}$$

(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 $\mathcal{E}_0$. Therefore the potential energy of the particle is,

$$V(x) = \frac{1}{2} m\omega_0 x^2 + q_m \mathcal{E}_0 \, x$$

(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,

$$\langle x \rangle(t) = \frac{q\mathcal{E}_0}{m\omega_0^2}(1 - \cos\omega_0 t) \qquad \langle p \rangle(t) = \frac{q\mathcal{E}_0}{\omega_0} \sin\omega_0 t \tag{2.40}$$

(c) Give the energy mean value $\langle H \rangle$.

Chapter 3

Two-level systems

3.1 Two-level systems

at this point one should talk about the magnetic and electric dipole moments, defined as below:

$$V_B(t) = -\mathbf{m} \cdot \mathcal{B}(t), \tag{3.1}$$

$$V_E(t) = -\mathbf{d} \cdot \mathcal{E}(t). \tag{3.2}$$

3.2 Time-evolution of a TLS.

Let's take a quantum system, characterized by its hamiltonian, op_0, with only two eigenstates $|\phi_1\rangle$, $|\phi_2\rangle$ with energies E_1 and E_2. Then for this system the following relations hold:

$$\hat{H}_0|\phi_i\rangle = E_i|\phi_i\rangle, \qquad i = 1, 2. \tag{3.3}$$

$$\langle\phi_i|\phi_j\rangle = \delta_{ij}, \qquad \sum_i |\phi_i\rangle\langle\phi_i| = \mathbb{1}. \tag{3.4}$$

Undistorted TLS (isolated).

If the system initially is initially in the state $|\psi_0\rangle$ it is straightforward to find its state some time later (provided that no measurement has been performed): [21]

[21] $c_i(t) = c_i(0)e^{-\imath E_i t/\hbar}, \qquad i = 1, 2$

$$|\psi_0\rangle = c_1(0)|\phi_1\rangle + c_2(0)|\phi_2\rangle \tag{3.5}$$

$$\Longrightarrow$$

$$|\psi(t)\rangle = c_1(0)e^{-\imath\frac{E_1}{\hbar}t}|\phi_1\rangle + c_2(0)e^{-\imath\frac{E_2}{\hbar}t}|\phi_2\rangle \tag{3.6}$$

One special case of the above is expressions is when the initial state is one of the system's eigenstate (e.g. say $|\phi_2\rangle$. In this case we have, $c_1(0) = 0$ and $c_2(0) = 1$ (since the states should be normalized and then,

$$|\psi(t)\rangle = e^{-\imath\frac{E_2}{\hbar}t}|\phi_2\rangle,$$

As it is has been shown according to QM $|\psi(t)\rangle$ and $|\phi_2\rangle$ represent the same state since they differ by a global phase factor of the form $e^{\imath\theta}$, with θ arbitrary real number (here $\theta = E_2/\hbar$). It's not difficult to see that the probability of an energy measurement to give energy E_2 (equal to unity) is constant in time:

$$P_{E=E_2}(t) = |c_2(t)|^2 = |c_2(0)e^{-\imath E_2/t}|^2 = |c_2(0)|^2 = 1 = P_{E=E_2}(0).$$

It's easy to see that they have the same length: [22]

[22] Recall the rule:

$|\psi\rangle = a|\phi\rangle \qquad \rightarrow \qquad \langle\psi| = \langle\phi|a^*$

$$\langle\psi(t)|\psi(t)\rangle = \left(\langle\phi_2|e^{\imath E_2 t/\hbar}\right)\left(e^{-\imath E_2 t/\hbar}|\phi_2\rangle\right) = \langle\phi_2|\phi_2\rangle = 1.$$

In other words, if the system is in one of its eigenstates, unless it is perturbed, will stay there for ever! [23]

[23] For this reason the Hamiltonian eigenstates are also known as 'stationary'.

Distorted TLS by a (weak) external field.

Let's know assume that the quantum system is distorted by an external interaction, represented by the operator $\hat{V}$ which in principle can be either time-dependent, $\hat{V}(t)$ or static $\hat{V}_0$, [24]. The condition that the external interaction should be 'weak' will be specified later in a quantitative context.

The question is, if the system is in state $|\psi_0\rangle$ how now the system's state develops in time?

In other words we need to find $|\psi(t)\rangle$. QM's answer is the TDSE law about the state's time-evolution,

$$\imath\hbar\frac{\partial}{\partial t}\psi(t) = [\hat{H}_0 + \hat{V}]\psi(t) \tag{3.7}$$

Also, we know that the time-dependent state may be written in terms of the $\hat{H}_0$ eigenbasis as,

$$|\psi(t)\rangle = c_1(t)|\phi_1\rangle + c_2(t)|\phi_2\rangle. \tag{3.8}$$

Since it is assumed that $|\phi_i\rangle$, $i = 1, 2$ are known, to calculate $|\psi(t)\rangle$ is equivalent to calculate the coefficients, $c_1(t)$ and $c_2(t)$. This is done by inserting our TLS's wavefunction into (3.7):

$$\imath\frac{\partial}{\partial t}\left[c_1(t)|\phi_1\rangle + c_2(t)|\phi_2\rangle\right] = (\hat{H}_0 + \hat{V})\left[c_1(t)|\phi_1\rangle + c_2(t)|\phi_2\rangle\right].$$

The next step is to multiply from the left with $\langle\phi_1|$ and $\langle\phi_2|$ from the left to obtain, [25]

$$\begin{aligned}
\imath\frac{d}{dt}\left[c_1(t)\langle 1|1\rangle + c_2(t)\langle 1|2\rangle\right] &= \langle 1|(\hat{H}_0 + \hat{V})\left[c_1(t)|1\rangle + c_2(t)|2\rangle\right] \\
\imath\frac{d}{dt}\left[c_1(t)\langle 2|1s\rangle + c_2(t)\langle 2|2\rangle\right] &= \langle 2|(\hat{H}_0 + \hat{V})\left[c_1(t)|1\rangle + c_2(t)|2\rangle\right],
\end{aligned}$$

where $\langle i|j\rangle = \langle\phi_i|\phi_j\rangle$. These equations simplify since, by definition $\langle 1|1\rangle = \langle 2|2\rangle = 1$, $\langle 1|2\rangle = 0$ and by noticing that,

$$\begin{aligned}
\langle 1|\hat{H}_0|1\rangle &= \langle 1|E_1|1\rangle = E_1\langle 1|1\rangle = E_1, \\
\langle 2|\hat{H}_0|2\rangle &= \langle 2|E_2|2\rangle = E_2\langle 2|2\rangle = E_2, \\
\langle 1|\hat{H}_0|2\rangle &= \langle 1|E_2|2\rangle = E_2\langle 1|2\rangle = 0 \\
\langle i|\hat{V}|i\rangle &= V_{ii}, \qquad i = 1, 2 \\
\langle 1|\hat{V}|2\rangle &= V_{12} \\
\langle 2|\hat{V}|1\rangle &= V_{21},
\end{aligned}$$

Substituting these value the following coupled system of ODEs is obtained:

[24] e.g for example one may think a particle with spin $s = 1/2$ in the presence of a magnetic field, $B(t)$ modelled as in (3.1) or an hydrogen in a electric field as in (3.2).

[25] To keep the notation simple we set:

$$|1\rangle \equiv |\phi_1\rangle, \qquad |2\rangle \equiv |\phi_2\rangle$$

$$\imath\dot{c}_1(t) = \omega_1 c_1(t) + \Omega_0\, c_2(t) \tag{3.9}$$
$$\imath\dot{c}_2(t) = \omega_2 c_2(t) + \Omega_0^*\, c_1(t), \tag{3.10}$$

where we have defined Rabi-frequency, Ω_0 and the eigen-frequencies, ω_i as, [26]

$$\omega_i = \frac{1}{\hbar}(E_i + V_{ii}), \qquad i = 1, 2, \tag{3.11}$$
$$\Omega_0 = \frac{V_{12}}{\hbar}. \tag{3.12}$$
$$\omega_0 = \omega_2 - \omega_1. \tag{3.13}$$

The later frequency based on the energy difference between the two states, ω_0, was defined for later convenience. At this point one can use any method to solve this system of equation. As first-order ODE, the solution is only possible when it is supplemented with the initial conditions for $c_1(t)$ and $c_2(t)$. For example, if the system is initially in its ground state which means that $P_{E=E_1}(0) = |c_1(0)| = 1$,

$$c_1(0) = 1, \quad c_2(0) = 0. \tag{3.14}$$

[27]

Constant interaction, $\hat{V}$. In this case ω_i, Ω_0 are also constants and the equations for $c_1(t)$ and $c_2(t)$ are ordinary differential equations (ODEs) with constant coefficients. There are few way that one can proceed further. One is to transform to another set of equations by setting,

$$c_1(t) = u_1(t)e^{-\imath\omega_1 t}, \qquad c_2(t) = u_2(t)e^{-\imath\omega_2 t} \tag{3.15}$$

Upon inserting these transformations into (3.9)-(3.10) we are left with:

$$\imath\dot{u}_1(t) = \Omega_0\, e^{-\imath\omega_0 t} u_2(t), \tag{3.16}$$
$$\imath\dot{u}_2(t) = \Omega_0^*\, e^{+\imath\omega_0 t} u_1(t). \tag{3.17}$$

We can decouple this coupled system of ODEs by taking the time derivative of the second equation and then insert the expression for $\dot{u}_1(t)$ (first equation) into said derivative resulting to a second-order ODE describing a damped *harmonic oscillator* (DHO): [28]

[26] Of course,

$$\Omega_0^* = \frac{V_{12}}{\hbar}$$

[27] Strictly, speaking we should choose $c_1(0) = e^{\imath\phi}$ and $c_2(0) = 0$, but one may set $c_1(0) = 1$ with no loss of generality, as the observables depend on the phase difference between $c_1(t)$ and $c_2(t)$ and not the absolute phases of each state separately.)

[28] Reminder for the DHO:

$$\ddot{x}(t) + \gamma\dot{x}(t) + \omega_0^2 x(t) = 0.$$

It's solution for $\omega < \gamma/2$ is

$$x(t) = e^{-\frac{\gamma t}{2}}\left[A_1 e^{-\alpha t} + A_2 e^{\alpha t}\right]$$

with A_1, A_2 determined through the initial conditions.

$$\ddot{u}_2 - \imath\omega_0\dot{u}_2 + |\Omega_0|^2 u_2 = 0. \tag{3.18}$$

Following the same procedure for the amplitude $u_1(t)$ we arrive at,

$$\ddot{u}_1 + \imath\omega_0\dot{u}_1 + |\Omega_0|^2 u_1 = 0. \tag{3.19}$$

Now the amplitude equations are decoupled and have the form of a DHO with damping parameter, $\imath\omega_0$ and 'eigen'-frequency, Ω_0! It's straightforward now to assume a solution of the form:

$$u_1(t) = Ae^{\sigma t},$$

which by substitution in (3.19) for the possible σ:

$$\sigma^2 + \imath\omega_0\sigma + |\Omega_0|^2\sigma = 0 \qquad \rightarrow$$
$$\sigma_{12} = \frac{-\imath\omega_0 \pm \sqrt{(\imath\omega_0)^2 - 4|\Omega_0|^2}}{2} = \imath\frac{\omega_0 \mp \sqrt{\omega_0^2 + 4|\Omega_0|^2}}{2} = \imath\frac{\omega_0 \mp \tilde{\Omega}}{2}$$

where the a modified Rabi-frequency has now appeared,

$$\boxed{\tilde{\Omega} = \sqrt{\omega_0^2 + 4|\Omega_0|^2}} \tag{3.20}$$

Eventually we find for $u_2(t)$ the general solution,

$$u_1(t) = e^{\imath\omega_0 t/2}\left(A_1 e^{\imath\tilde{\Omega}/2} + A_2 e^{-\imath\tilde{\Omega}/2}\right). \tag{3.21}$$

For the $u_2(t)$ amplitude we find a similar equation as,

$$u_2(t) = e^{-\imath\omega_0 t/2}\left(B_1 e^{\imath\tilde{\Omega}/2} + B_2 e^{-\imath\tilde{\Omega}/2}\right). \tag{3.22}$$

The exact form of the solution depends on the initial state. In the present case, two initial conditions needs to be set (since we have two unknown constants).

Case: Initial state of the system $|\phi_1\rangle$. Assuming the system initially in this state and recalling (3.17), we have[1],

$$u_1(0) = 1 \qquad \rightarrow \qquad \dot{u}_2(0) = -\imath\Omega_0^*(0).$$

So, we are going to specialize the general solution for $u_2(t)$ (3.22) with initial conditions:

$$\boxed{u_2(0) = 0, \qquad \dot{u}_2(0) = -\imath\Omega_0^*(0).}$$

[1]The initial conditions may be defined within an arbitrary phase constant. Any value of $u_1(0)$ is a legitimate one, as long as $|u_1(0)|^2 + |u_2(0)|^2 = 1$.

Given the initial conditions, the solution is expressed as,

$$u_2(t) = -\frac{2\imath\Omega_0^*}{\tilde{\Omega}} e^{\imath\omega_0 t/2} \sin(\frac{\tilde{\Omega}t}{2}) \tag{3.23}$$

With $u_2(t)$ known, $u_1(t)$ can be found by substituting (3.23) into (**??**) followed by integration from $t' = 0$ to a $t > 0$:

$$u_1(t) = e^{-\imath\omega_0 t/2} \left[\cos(\frac{\tilde{\Omega}t}{2}) + \imath \frac{\omega_0}{\tilde{\Omega}} \sin(\frac{\tilde{\Omega}t}{2}) \right] \tag{3.24}$$

Given the above solutions the probability of the system, upon energy measurement, is given by, [29]

$$P_{E=E_2}(t) = |c_2(t)|^2 = \frac{4|\Omega_0|^2}{|\tilde{\Omega}|^2} \sin^2(\frac{\tilde{\Omega}t}{2}),$$
$$P_{E=E_2}(t) = 1 - |c_2(t)|^2 = 1 - \frac{4|\Omega_0|^2}{|\tilde{\Omega}|^2} \sin^2(\frac{\tilde{\Omega}t}{2}).$$

Finally, having the $u_i(t), i = 1, 2$ available the $c_i(t)$ can be found from (3.15) and from (3.8) the TD wavefunction $\psi(\mathbf{r}, t)$ results to,

$$|\psi(t)\rangle = \frac{2e^{-\imath(\epsilon_1+\epsilon_2)t/2}}{\tilde{\Omega}} [\Omega_0 \cos(\frac{\tilde{\Omega}t}{2} - \bar{\phi})|\phi_1\rangle - \imath\Omega_0^* \sin(\frac{\tilde{\Omega}t}{2})|\phi_2\rangle].$$

with $\bar{\phi}$ defined by, $\tilde{\Omega} = 2\Omega_0^* \cos\bar{\phi}$ and $\imath\delta = 2\Omega_0^* \sin\bar{\phi}$. A quick observation is that an off-resonant excitation shortens the oscillation

to be continued...

[29] Note that,

$$|c_i(t)|^2 = |u_i(t)|^2, \quad i = 1, 2$$