

1. Basic Quantum Mechanics

“Quantum phenomena do not occur in a Hilbert space, they occur in a laboratory.”

– Asher Peres, Quantum Theory: Concepts and Methods.

1.1 Mathematical Preliminaries

A physical state is represented mathematically by a vector in a Hilbert space. Physical observables are represented by operators acting in the space of states. We recap here, the essential properties of Hilbert spaces, in the case of finite dimension.

1.1.1 Linear vector space

Note 1.1.1 Linear vector spaces.

A linear vector space is a set of elements, called vectors, which is closed under addition and multiplication by scalars. Using Dirac notation, the vectors are denoted by kets: $|\psi\rangle$. We can associate to each ket a vector in the dual space called bra: $\langle\psi|$.

If two vectors $|\psi\rangle$ and $|\phi\rangle$ are part of a vector space, then $|\psi\rangle + |\phi\rangle$ also belongs to the space. If a vector $|\psi\rangle$ is in the space, then $\alpha|\psi\rangle$ is also in the space (where α is a complex scalar).

The bra dual to $c|\psi\rangle$ is $c^* \langle\psi|$.

A set of linearly independent vectors $\{|\psi_i\rangle\}$ is such that $\sum_k c_k |\psi_k\rangle = 0$ if and only if $c_k = 0, \forall k$ (i.e. no trivial combination of them sums to zero). The dimension of the space d is the maximum number of linearly independent vectors (which is also the smallest number of vectors that span the space).

Note 1.1.2 Basis.

A maximal set of linearly independent vectors in the space is called a basis. (e.g. $\{|\phi_k\rangle, k = 1, \dots, d\}$). Any vector in the space can be written as a linear superposition of the basis vectors: $|\psi\rangle = \sum_k a_k |\phi_k\rangle$. To any vector we can thus associate a column vector of d complex numbers $(a_1, a_2 \dots a_d)^T$. We will restrict ourselves to bounded, finite dimension spaces (even if many physical spaces are not, e.g. energy spaces can be unbounded and position has infinite dimension).

Note 1.1.3 Hilbert space.

The Hilbert space is a linear vector space over complex numbers with an inner product.

Note 1.1.4 Inner product.

An inner product is an ordered mapping from two vectors to a complex number. For a Hilbert space, the inner product is a mapping from a ket and a bra to a complex number $c = \langle \psi | \phi \rangle$ with the following properties:

- *positivity*: $\langle \psi | \psi \rangle \geq 0$. The equality holds only for the zero vector $|\psi\rangle = 0$.
- *skew symmetry*: $\langle \psi | \phi \rangle = \langle \phi | \psi \rangle^*$.
If $|\phi\rangle = c_1 |\phi_1\rangle + c_2 |\phi_2\rangle$, then
- *linearity (of kets)*: $\langle \psi | \phi \rangle = c_1 \langle \psi | \phi_1 \rangle + c_2 \langle \psi | \phi_2 \rangle$, and
- *anti-linearity (of bras)*: $\langle \phi | \psi \rangle = c_1^* \langle \phi_1 | \psi \rangle + c_2^* \langle \phi_2 | \psi \rangle$.

Note 1.1.5 Norm.

The norm of a vector is $\| |\psi\rangle \| = \sqrt{\langle \psi | \psi \rangle}$. Since the Hilbert space is characterized by its inner product, vectors are defined up to a global phase, i.e. if $|\phi\rangle = e^{i\theta} |\psi\rangle$ then $\langle \phi | \phi \rangle = \langle \psi | \psi \rangle$ and the vectors $|\phi\rangle$ and $|\psi\rangle$ are indistinguishable. Instead, relative phase is of huge importance: $|\phi\rangle + e^{i\theta} |\psi\rangle \neq |\phi\rangle + |\psi\rangle$.

The inner product properties allow us to define two geometric inequalities:

- *Schwartz inequality*: $|\langle \psi | \phi \rangle|^2 \leq \langle \psi | \psi \rangle \langle \phi | \phi \rangle$.
- *Triangular inequality*: $\| |\psi\rangle + |\phi\rangle \| \leq \| |\psi\rangle \| + \| |\phi\rangle \|$.

The equality holds only if the two vectors are in the same direction: $|\psi\rangle = c |\phi\rangle$.

Note 1.1.6 Orthonormal set.

A set of vectors $\{|\psi_k\rangle\}$ is orthonormal if for each pair the inner product $\langle \psi_i | \psi_j \rangle = \delta_{ij}$, where the Kronecker delta is given by

$$\delta_{ij} = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{if } i \neq j. \end{cases} \quad (1.1)$$

1.1.2 Operators

Note 1.1.7 Operator.

An operator \hat{A} on a vector space is a mapping between two vectors in that space: $\hat{A} |\psi\rangle = |\phi\rangle$. A linear operator satisfies:

$$\hat{A}(c_1 |\psi_1\rangle + c_2 |\psi_2\rangle) = c_1 \hat{A} |\psi_1\rangle + c_2 \hat{A} |\psi_2\rangle. \quad (1.2)$$

To characterize and parametrize \hat{A} we look at its action on each vector in the space. Because of linearity, it is enough to characterize \hat{A} with its action on the basis vectors. In this way we can associate a matrix representation to any operator, in the same way we associated arrays of complex numbers with the vectors.

In particular, given an orthonormal basis $\{|\psi_k\rangle\}$, the matrix representation of the operator \hat{A} is an $d \times d$ square matrix whose elements are given by $A_{ij} = \langle \psi_i | \hat{A} | \psi_j \rangle$.¹

Let us consider an orthonormal basis $\{|\psi_i\rangle\}$, then any vector can be written as some linear combination of the basis vectors: $|\psi\rangle = \sum_{j=1}^d a_j |\psi_j\rangle$ and $|\phi\rangle = \sum_{k=1}^d b_k |\psi_k\rangle$. The action of an operator \hat{A} that is given by

$$\begin{aligned} \hat{A} |\psi\rangle &= |\phi\rangle \\ \implies \sum_{j=1}^d \hat{A} a_j |\psi_j\rangle &= \sum_{k=1}^d b_k |\psi_k\rangle. \end{aligned} \quad (1.3)$$

¹Read A_{ij} as the entry on the i -th row and j -th column of matrix \hat{A} . It should be unambiguous from the context that \hat{A} (with hat, without subscripts) denote the matrix or operator while A_{ij} (with subscripts) denote the (i, j) -th matrix element. At later points in the lecture notes, I drop the hat for notational convenience, but it should be clear from the context what the notation means.

To extract one of the coefficients, e.g. b_i , we multiply by the corresponding bra $\langle v_i |$ to obtain

$$\begin{aligned} \sum_{j=1}^d \langle v_i | \hat{A} a_j | v_j \rangle &= \sum_{k=1}^d \langle v_i | b_k | v_k \rangle \\ \sum_{j=1}^d a_j \underbrace{\langle v_i | \hat{A} | v_j \rangle}_{A_{ij}} &= \sum_{k=1}^d b_k \underbrace{\langle v_i | v_k \rangle}_{\delta_{ik}} \\ \implies \sum_{j=1}^d A_{ij} a_j &= b_i \end{aligned} \quad (1.4)$$

From the final line above, the action of an operator can be thus seen as a matrix multiplication (again, here we are restricting to bounded, finite dimension spaces that support finite operators, hence this simple matrix representation).

■ **Example 1.1** An operator in matrix representation is given by

$$A = \begin{pmatrix} -1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{pmatrix}. \quad (1.5)$$

It acts on a vector

$$v = \begin{pmatrix} 1/\sqrt{3} \\ 1/\sqrt{3} \\ -1/\sqrt{3} \end{pmatrix} \quad (1.6)$$

to give

$$Av = b_1 \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + b_2 \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} + b_3 \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \quad (1.7)$$

Find the coefficients b_i .

1.1.3 Hermitian operators

Note 1.1.8 Adjoint operation. The adjoint of an operator \hat{A} is denoted with a “dagger” symbol: \hat{A}^\dagger . It is an operator acting on the dual space (i.e. the bra vector) with the property:

$$\langle (\hat{A}^\dagger \psi) | \phi \rangle = \langle \psi | (\hat{A} \phi) \rangle, \forall |\psi\rangle, |\phi\rangle. \quad (1.8)$$

We can also have other notations. From $\langle \phi | \psi \rangle = \langle \psi | \phi \rangle^*$, (where $*$ indicates the complex conjugate), we have $\langle (\hat{A}^\dagger \psi) | \phi \rangle = \langle \psi | (\hat{A} \phi) \rangle = \langle \phi | \hat{A}^\dagger \psi \rangle^*$. Importantly, we can write the inner product as $\langle \phi | (\hat{A} \psi) \rangle = \langle \phi | \hat{A} | \psi \rangle$ and $\langle (\hat{A} \phi) | \psi \rangle = \langle \phi | \hat{A}^\dagger | \psi \rangle$.

In matrix representation, this means that the adjoint of an operator is the *conjugate transpose* of that operator, i.e.

$$(\hat{A}^\dagger)_{ij} = \langle i | \hat{A}^\dagger | j \rangle = \langle j | \hat{A} | i \rangle^* = (\hat{A}^*)_{ji}. \quad (1.9)$$

Note 1.1.9 Self-adjoint or Hermitian. A self adjoint or Hermitian operator is an operator such that \hat{A} and \hat{A}^\dagger operate on the same domain and with the property $\langle \psi | \hat{A} | \phi \rangle = \langle \phi | \hat{A} | \psi \rangle^*$, or in matrix representation $A_{ij} = A_{ji}^*$. In short, $\hat{A} = \hat{A}^\dagger$.

Also, Hermitian operators have the following useful properties.

Properties of Hermitian operators

1. Every Hermitian operator of dimension d always has d (not necessarily distinct) **real** eigenvalues.
2. The corresponding d eigenvectors can always be chosen to form an orthonormal basis.

■ **Example 1.2** Show that Hermitian operators have real eigenvalues (property 1). ■

■ **Example 1.3** Prove that $(c\hat{A})^\dagger = c^* \hat{A}^\dagger$. ■

■ **Example 1.4** Prove that $(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger \hat{A}^\dagger$. ■

■ **Example 1.5** Prove that $(\hat{A}\hat{B} + \hat{B}\hat{A})^\dagger = \hat{B}^\dagger \hat{A}^\dagger + \hat{A}^\dagger \hat{B}^\dagger = \hat{B}\hat{A} + \hat{A}\hat{B}$. ■

1.1.4 Properties of Operators

Note 1.1.10 Outer Product. The outer product, $|\psi\rangle\langle\phi|$ is an operator. This can be seen from its operation on a ket vector, which returns another ket vector: $(|\psi\rangle\langle\phi|)|\alpha\rangle = |\psi\rangle(\langle\phi|\alpha)$.

A projection operator is defined as

$$\hat{P}_i = |i\rangle\langle i|. \quad (1.10)$$

For any basis set, the sum over all projectors on the vector space is the identity,

$$\sum_i |i\rangle\langle i| = \mathbb{I}. \quad (1.11)$$

The product of two projectors is $\hat{P}_i\hat{P}_j = \delta_{ij}\hat{P}_i$.

Note 1.1.11 Trace. The trace of an operator is the sum of the diagonal elements,

$$\text{Tr}(\hat{A}) = \sum_i A_{ii}. \quad (1.12)$$

It is independent of the choice of basis.

Note 1.1.12 Spectral Theorem.

Spectral theorem

Given a self-adjoint (Hermitian) operator \hat{A} on a linear vector space \mathcal{H} , there exists an orthonormal basis of \mathcal{H} consisting of the eigenvectors of \hat{A} . Consequently, \hat{A} can be written as a linear combination of pairwise orthogonal projections formed from its eigenvectors. This representation is called the *spectral decomposition*:

$$\hat{A} = \sum_j a_j |v_j\rangle\langle v_j|, \quad \text{where } \hat{A}|v_j\rangle = a_j |v_j\rangle. \quad (1.13)$$

In this basis, the matrix representation of \hat{A} is diagonal.

The spectral theorem is a theorem of fundamental importance in quantum mechanics, upon which the statistical interpretation of quantum mechanics is based.

Theorem

If two self-adjoint (Hermitian) operators \hat{A}, \hat{B} commute, then they share a common set of eigenvectors.

Proof:

Operators \hat{A}, \hat{B} are Hermitian $\Rightarrow \hat{A}^\dagger = \hat{A}$ and $\hat{B}^\dagger = \hat{B}$.

Given $|a\rangle, |a'\rangle$ are eigenvectors of \hat{A} , with respective eigenvalues a, a' ,

$$\text{if } [\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} = 0,$$

$$\text{then } \langle a|(\hat{A}\hat{B} - \hat{B}\hat{A})|a'\rangle = 0$$

$$\Rightarrow \langle a|(\hat{A}^\dagger\hat{B} - \hat{B}\hat{A})|a'\rangle = 0$$

$$\Rightarrow a\langle a|\hat{B}|a'\rangle - a'\langle a|\hat{B}|a'\rangle = 0$$

$$\Rightarrow (a - a')\langle a|\hat{B}|a'\rangle = 0$$

$$\begin{aligned} & \text{either } a - a' \neq 0, \\ & \quad \langle a|\hat{B}|a'\rangle = 0 \quad \Rightarrow \text{off-diagonal elements of } \hat{B} \text{ are zero} \\ & \quad \text{i.e. } \hat{B} \text{ shares simultaneous eigenvectors with } \hat{A} \\ & \text{or } a - a' = 0, \\ & \quad a = a' \quad \Rightarrow \text{diagonal elements } \langle a|\hat{B}|a\rangle \text{ can be zero or non-zero} \\ & \quad \text{(But is not central to our argument.)} \end{aligned} \tag{1.14}$$

1.1.5 Unitary operators

An operator \hat{U} is unitary if

$$\hat{U}\hat{U}^\dagger = \hat{U}^\dagger\hat{U} = \mathbb{I}. \tag{1.15}$$

Unitary operators preserve the norm of vectors: if $|\psi'\rangle = \hat{U}|\psi\rangle$ then $\||\psi'\rangle| = \||\psi\rangle|$. Unitary operations are the complex version of rotation operations: when a vector is rotated, its length does not change. More importantly, unitary operations appear naturally when diagonalizing matrices.

Given a set of d eigenvectors $\{|\lambda_i\rangle\}$ of a Hermitian operator \hat{A} which form an orthonormal basis, and another orthonormal basis set $\{|i\rangle\}$ which span the same space, define the unitary operator

$$\hat{U} = \sum_{i=1}^d |\lambda_i\rangle\langle i|. \tag{1.16}$$

Then, the entries of the operator \hat{U} in matrix form, using the basis $|i\rangle$, is $U_{ij} = \langle i|\hat{U}|j\rangle$, and they are such that the eigenvectors $|\lambda_i\rangle$ are arranged column-wise:

$$\hat{U} = \begin{pmatrix} \vdots & \vdots & \cdots & \vdots \\ \vdots & \vdots & \cdots & \vdots \\ |\lambda_1\rangle & |\lambda_2\rangle & \cdots & |\lambda_d\rangle \\ \vdots & \vdots & \cdots & \vdots \\ \vdots & \vdots & \cdots & \vdots \end{pmatrix}. \tag{1.17}$$

When applied in this manner, $\hat{U}^\dagger \hat{A} \hat{U} \equiv \hat{\Lambda}$ is a diagonal matrix, as shown below.

$$\begin{aligned}\hat{U}^\dagger \hat{A} \hat{U} &= \sum_{i,j=1}^d |i\rangle \underbrace{\langle \lambda_i | \hat{A} | \lambda_j \rangle}_{=\lambda_j \langle \lambda_i | \lambda_j \rangle = \lambda_j \delta_{ij}} \langle j| \\ &= \sum_i \lambda_i |i\rangle \langle i| \\ &= \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_d).\end{aligned}\quad (1.18)$$

Consequently,

$$\hat{\Lambda} \equiv \hat{U}^\dagger \hat{A} \hat{U} \Leftrightarrow \hat{A} = \hat{U} \hat{\Lambda} \hat{U}^\dagger.\quad (1.19)$$

Any Hermitian matrix may be diagonalized by a unitary transformation.

■ **Example 1.6** In the previous example, the operator A is given in matrix form, by

$$A = \begin{pmatrix} -1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{pmatrix}.\quad (1.20)$$

Diagonalize this matrix. Recall the procedure for diagonalization:

1. Find the characteristic polynomial.
2. Solve for the eigenvalues.
3. Put each eigenvalue back into the characteristic equation to solve for eigenvectors.
4. Construct the unitary transformation (for Hermitian matrices).

■

1.1.6 Function of an Operator

Let $f(x)$ be an arbitrary function, e.g. $\exp(x)$, with a Taylor series expansion, $f(x) = \sum_n c_n x^n$, for some coefficients c_n .

We define the application of the function on an operator, $f(\hat{A})$, by

$$f(\hat{A}) := \sum_{n=0}^{\infty} c_n \hat{A}^n.\quad (1.21)$$

This is only easy to compute if the operator is diagonal.

Consider a Hermitian operator \hat{A} , which has a spectral decomposition $\hat{A} = \sum_i \lambda_i |\lambda_i\rangle \langle \lambda_i|$. Since Hermitian operators have eigenvectors that are orthonormal, $\langle \lambda_i | \lambda_j \rangle = \delta_{ij}$. We therefore get

$$\hat{A}^2 = \hat{A} \hat{A} = \sum_i \lambda_i |\lambda_i\rangle \langle \lambda_i| \sum_j \lambda_j |\lambda_j\rangle \langle \lambda_j| = \sum_i \lambda_i^2 |\lambda_i\rangle \langle \lambda_i|,\quad (1.22)$$

$$\hat{A}^3 = \hat{A} \hat{A}^2 = \dots = \sum_i \lambda_i^3 |\lambda_i\rangle \langle \lambda_i|,\quad (1.23)$$

$$\hat{A}^n = \sum_i \lambda_i^n |\lambda_i\rangle \langle \lambda_i|.\quad (1.24)$$

Inserting these into Eq. (1.21), we get

$$\begin{aligned}f(\hat{A}) &= \sum_{n=0}^{\infty} c_n \sum_i \lambda_i^n |\lambda_i\rangle \langle \lambda_i| = \sum_i \left(\sum_n c_n \lambda_i^n \right) |\lambda_i\rangle \langle \lambda_i| \\ &= \sum_i f(\lambda_i) |\lambda_i\rangle \langle \lambda_i|.\end{aligned}\quad (1.25)$$

That means, the function acts only on the eigenvalues λ_i of the operator \hat{A} in its eigenbasis.

■ **Example 1.7** The Pauli- z operator is given by $\hat{\sigma}_z = |0\rangle\langle 0| - |1\rangle\langle 1|$, which is diagonal. Compute $\exp(i\theta\hat{\sigma}_z)$.

Of course, the result (Eq. (1.25)) is useful only if \hat{A} is diagonal, which in general, it need not be. Now consider that \hat{A} is not diagonal, but is related to the diagonal operator \hat{B} , by a unitary transformation, $\hat{A} = \hat{U}\hat{B}\hat{U}^\dagger$. Then,

$$\hat{A}^2 = \hat{A}\hat{A} = (\hat{U}\hat{B}\hat{U}^\dagger)(\hat{U}\hat{B}\hat{U}^\dagger) = \hat{U}\hat{B}^2\hat{U}^\dagger, \quad (1.26)$$

$$\hat{A}^n = \hat{U}\hat{B}^n\hat{U}^\dagger. \quad (1.27)$$

Thus,

$$\begin{aligned} f(\hat{A}) &= \sum_{n=0}^{\infty} c_n \hat{A}^n = \sum_{n=0}^{\infty} c_n \hat{U}\hat{B}^n\hat{U}^\dagger = \hat{U} \left(\sum_{n=0}^{\infty} c_n \hat{B}^n \right) \hat{U}^\dagger \\ &= \hat{U}f(\hat{B})\hat{U}^\dagger. \end{aligned} \quad (1.28)$$

Therefore, we can compute $f(\hat{A})$ because we know (i) \hat{A} 's transformation from \hat{B} , and (ii) how to compute the function of a diagonal operator.

■ **Example 1.8** The Pauli- x operator is not diagonal: $\hat{\sigma}_x = |0\rangle\langle 1| + |1\rangle\langle 0|$. It is related to $\hat{\sigma}_z$ by a unitary transformation, $\hat{\sigma}_x = \hat{U}\hat{\sigma}_z\hat{U}^\dagger$, where $\hat{U} = \frac{1}{\sqrt{2}}(|0\rangle\langle 0| + |0\rangle\langle 1| + |1\rangle\langle 0| - |1\rangle\langle 1|)$. Clearly, $\hat{U}^\dagger = \hat{U}$. Compute $\exp(i\theta\hat{\sigma}_x)$.

1.2 Postulates of Quantum Mechanics (Pure states)

There are four main postulates that quantum mechanics can be built upon.

Postulate 1 : Description of the state of a system.

To any physical system we can associate an abstract, complex vector space with an inner product, known as a **Hilbert space** \mathcal{H} , such that the state of the system at any given instant in time t can be described by a vector $|\psi(t)\rangle$ in this space. Vectors in the state space can be expanded in a linear combination of orthonormal basis vectors $|k\rangle$, e.g. $|v\rangle \equiv \sum_k v_k |k\rangle$. They have dual vectors $\langle v| = |v\rangle^\dagger$ and are normalized $\| |v\rangle \| = \sqrt{\langle v|v \rangle} = 1$. The inner product is $\langle v|w\rangle = \sum_k v_k^* w_k$ and the outer product forms an operator $|v\rangle\langle w|$.

Postulate 2 : Combining quantum systems.

Given two quantum systems with respective Hilbert spaces \mathcal{H}_1 and \mathcal{H}_2 , the combined quantum system has a Hilbert space associated with it given by $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$.

The dimension of the composite Hilbert space is $d = d_1 \times d_2$, and the d vectors are denoted by the ordered pairs $|v_i\rangle \otimes |w_j\rangle$ (also written as $|v_i, w_j\rangle$) where $|v_i\rangle \in \mathcal{H}_1, |w_j\rangle \in \mathcal{H}_2$. The inner product on \mathcal{H} is given by $\langle v_i, w_j | v_k, w_l \rangle = \langle v_i | v_k \rangle \langle w_j | w_l \rangle$.

Postulate 3 : Time evolution (dynamics).

The time evolution of a closed system is described by a unitary transformation, $\hat{U}(t, t_0)$ on the initial state $|\psi(t_0)\rangle$, such that the state at a later time t is

$$|\psi(t)\rangle = \hat{U}(t, t_0) |\psi(t_0)\rangle, \quad (1.29)$$

where $\hat{U}(t, t_0)$ satisfies a differential equation,

$$i\hbar \frac{\partial}{\partial t} \hat{U}(t, t_0) = \hat{H} \hat{U}(t, t_0). \quad (1.30)$$

Here, \hat{H} is a Hermitian operator associated with the total energy of the system called the Hamiltonian.

Equivalently, the state vector of the closed system satisfies the Schrödinger equation

$$i\hbar \frac{\partial |\psi(t)\rangle}{\partial t} = \hat{H} |\psi(t)\rangle. \quad (1.31)$$

That the time evolution of a quantum state is unitary comes from the condition of probability conservation; unitary transformations preserve the norm of the state vector. See Sakurai Chap. 2.1 for a more detailed explanation.

The fourth postulate concerns measurement. Measurement in quantum mechanics is still an area of active debate.² We shall skip the issues for now and assume the validity of this next postulate. But first, we first motivate it with a simple example.

From PH2101 QM1, we are taught that given a quantum state

$$|\psi\rangle = a|0\rangle + b|1\rangle, \quad (1.32)$$

the Born rule states that the probability of measuring the state to be in $|0\rangle$ is $|a|^2$ and in $|1\rangle$ is $|b|^2$. If we had wanted to measure the state to be in some other orthogonal basis, say $|\pm\rangle \equiv \frac{1}{\sqrt{2}}(|0\rangle \pm |1\rangle)$, then we could rewrite the state as

$$|\psi\rangle = \frac{a+b}{\sqrt{2}}|+\rangle + \frac{a-b}{\sqrt{2}}|-\rangle, \quad (1.33)$$

and find the corresponding probabilities, $\frac{1}{2}|a \pm b|^2$ that the system is in states $|\pm\rangle$. But this is a little clumsy. Instead we will define a more rigorous mathematical formalism in the fourth postulate that is applicable to generalized measurement (applicable when the system is open, and when measurements are imperfect) and the special case of projective measurement (which can be thought of as ideal, perfect measurements on closed systems).

Postulate 4 Measurement (von Neumann scheme)

Quantum measurements are described by a collection $\{\hat{M}_k\}$ of measurement operators. These are operators acting on the state space of the system being measured. The index k refers to the measurement outcomes that may occur in the experiment. If the state of the quantum system is $|\psi\rangle$ immediately before the measurement then the probability that result k occurs is given by

$$p_k = \langle\psi|\hat{M}_k^\dagger\hat{M}_k|\psi\rangle = \|\hat{M}_k|\psi\rangle\|^2 \geq 0, \quad (1.34)$$

and the state after measurement is

$$|\psi\rangle \rightarrow \frac{\hat{M}_k|\psi\rangle}{\sqrt{\langle\psi|\hat{M}_k^\dagger\hat{M}_k|\psi\rangle}}. \quad (1.35)$$

This is the “wavefunction collapse” postulate. Here, the denominator is required for normalization of probabilities. The measurement operators satisfy the *completeness relation*,

$$\sum_k \hat{M}_k^\dagger\hat{M}_k = I, \quad (1.36)$$

which expresses the fact that probabilities sum to one:

$$1 = \sum_k p_k = \sum_k \langle\psi|\hat{M}_k^\dagger\hat{M}_k|\psi\rangle. \quad (1.37)$$

²Wikipedia (Measurement in quantum mechanics): *Many debates in the area known as quantum foundations concern the role of measurement in quantum mechanics. Recurring questions include which interpretation of probability theory is best suited for the probabilities calculated from the Born rule; and whether the apparent randomness of quantum measurement outcomes is fundamental, or a consequence of a deeper deterministic process. Worldviews that present answers to questions like these are known as “interpretations” of quantum mechanics.*

The collapse of the wavefunction is a source of confusion and contradictions: as stated above it appears as an almost instantaneous evolution of the system from a given state to another one, an evolution which is not unitary (as evolution should be, per Postulate 3). The source of contradiction stems from the fact that in this simple description of the measurement, the observer (or the measurement apparatus) are external to the system (thus the assumption of closed system is not respected) and might not even be quantum-mechanical.

On the other hand, we note that operationally the wavefunction collapse is required to define a well-formulated theory. The collapse allows the experimenter to check the result of the measurement by repeating it (on the system just observed) thus giving confidence on the measurement apparatus and procedure. If this were not the case, no measurement could be ever believed to be the correct one, so no confirmation of the theory could be done.

1.2.1 Special case: Projective Measurements

A projective measurement is described by an observable \hat{M} , a Hermitian operator on the state space of the system being observed. The observable has a spectral decomposition,

$$\hat{M} = \sum_k k \hat{P}_k, \quad (1.38)$$

where $\hat{P}_k \equiv |k\rangle\langle k|$ is a projection operator onto the eigenspace of \hat{M} with real eigenvalue k . Given a state $|\psi\rangle$, the possible outcomes of the measurement correspond to eigenvalues k , with probability p_k given by

$$p_k = \langle \psi | \hat{P}_k | \psi \rangle. \quad (1.39)$$

Given an outcome k that occurred (i.e. was measured), the state immediately after measurement is

$$|\psi\rangle \rightarrow \frac{\hat{P}_k |\psi\rangle}{\sqrt{p_k}}. \quad (1.40)$$

■ **Example 1.9** A simple but important example of a measurement is the measurement of a qubit in the computational basis. This is a measurement on a single qubit with two outcomes defined by the two measurement operators, $\hat{M}_0 = |0\rangle\langle 0|$, $\hat{M}_1 = |1\rangle\langle 1|$. Each measurement operator is Hermitian, and $\hat{M}_0^2 = \hat{M}_0$, $\hat{M}_1^2 = \hat{M}_1$, and they obey the completeness relation $\hat{M}_0^\dagger \hat{M}_0 + \hat{M}_1^\dagger \hat{M}_1 = \mathbb{I}$.

Suppose the state being measured is $|\psi\rangle = a|0\rangle + b|1\rangle$. Use the fourth postulate to find the probabilities of measuring $|0\rangle$ and $|1\rangle$ and the states after the measurement.

1.2.2 Measurement statistics

Although the result of an individual measurement or experiment is indeterminate, we can still calculate statistics of measurements. The average or expectation value of an observable \hat{A} measured on a system $|\psi\rangle$ is

$$\langle \hat{A} \rangle = \langle \psi | \hat{A} | \psi \rangle. \quad (1.41)$$

Uncertainty and Commutation Relations

- **Compatible Observables.** Two observables \hat{A} , \hat{B} are said to be *compatible* if their corresponding operators commute, $[\hat{A}, \hat{B}] = 0$, and incompatible otherwise.
- **Degeneracy.** If there exist two (or more) eigenstates of an operator A with the same eigenvalues, they are called degenerate.
- **Variance.** We define an operator $\Delta \hat{A} = \hat{A} - \langle \hat{A} \rangle$ for any observable \hat{A} . The expectation value of its square is the variance of \hat{A} , given by $\langle \Delta \hat{A}^2 \rangle = \langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2$.
- **Uncertainty Relation.** For any two observables, we have

$$\langle \Delta \hat{A}^2 \rangle \langle \Delta \hat{B}^2 \rangle \geq \frac{1}{4} \left| \langle [\hat{A}, \hat{B}] \rangle \right|^2 \quad (1.42)$$

1.3 Time Evolution of Closed Quantum Systems

Recall Postulate 3, where time evolution of a state ket is governed by a unitary operator such that

$$|\psi(t)\rangle = \hat{U}(t, t_0) |\psi(t_0)\rangle, \quad (1.43)$$

where the arguments in the operator denote the initial and final times t_0 and t respectively. The unitary operator obeys

$$i\hbar \frac{\partial}{\partial t} \hat{U}(t, t_0) = \hat{H} \hat{U}(t, t_0), \quad (1.44)$$

where H is the Hamiltonian. The time-evolution operator obeys the composition property

$$\hat{U}(t, t_0) = \hat{U}(t, t_1) \hat{U}(t_1, t_0), \text{ where } t_0 < t_1 < t. \quad (1.45)$$

Note that the composition sequence is read right to left, as should be the case for operators.

The formal solution to $\hat{U}(t, t_0)$ may be classified into three cases.

Time Evolution of Closed Quantum Systems

1. Case 1: \hat{H} is time-independent.

$$\hat{U}(t, t_0) = \exp \left\{ -\frac{i}{\hbar} \hat{H}(t - t_0) \right\}. \quad (1.46)$$

2. Case 2: \hat{H} is time-dependent, and commutes with itself at all times.

$$\hat{U}(t, t_0) = \exp \left\{ -\frac{i}{\hbar} \int_{t_0}^t \hat{H}(t') dt' \right\}. \quad (1.47)$$

3. Case 3: \hat{H} is time-dependent, and does not commute with itself at different times.

The solution is the Dyson series, which we shall not go into in this course.

$$\hat{U}(t, t_0) = \mathbb{I} + \sum_{n=0}^{\infty} \left(-\frac{i}{\hbar} \right)^n \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n \hat{H}(t_1) \hat{H}(t_2) \cdots \hat{H}(t_n). \quad (1.48)$$

The time-evolution operator reduces to the identity operator in the limit $\delta t \rightarrow 0$. Checking the exponentiated series for the time-independent case, indeed this is true: $\lim_{\delta t \rightarrow 0} \hat{U}(t + \delta t, t) = \lim_{\delta t \rightarrow 0} (\mathbb{I} - \frac{i}{\hbar} \hat{H} \delta t + \dots) = \mathbb{I}$.

A two level system is the simplest, non-trivial system in quantum mechanics that illustrates many characteristics of QM. Furthermore, it describes many simple physical systems, including quantum bits (qubits) – the building block of a quantum computer.

The canonical example of a two level system is a spin-1/2 particle, whose the time evolution is generated by the spin angular momentum operator. We make a small digression here to recall the properties of angular momentum in quantum mechanics before we come back to the topic of time-evolution of two level systems.

1.3.1 QM angular momentum as the generator of rotation

Recall, from PH3101, that a rotation in quantum mechanics is a unitary transformation. We know from classical mechanics that angular momentum is the generator of rotation. We therefore define the angular momentum operator³ \vec{J} such that an infinitesimal rotation of angle $\delta\phi$ around an axis \hat{n} is given by

$$U_n(\delta\phi) = \mathbb{I} - \frac{i}{\hbar} \delta\phi \vec{J} \cdot \hat{n}. \quad (1.49)$$

³From this point in this chapter, the hat on operators is dropped for convenience.

A finite rotation can be found by repeating many infinitesimal rotations. For example, for a rotation of angle ϕ about z is given by N repeats of rotation of angle $\delta\phi = \phi/N$, where $N \rightarrow \infty$:

$$\begin{aligned} U_z(\phi) &= \lim_{N \rightarrow \infty} \left(\mathbb{I} - \frac{i}{\hbar} \frac{\phi}{N} J_z \right)^N \\ &= \lim_{N \rightarrow \infty} \left[\mathbb{I} - N \left(\frac{iJ_z\phi}{N\hbar} \right) + \frac{N(N-1)}{2!} \left(\frac{iJ_z\phi}{N\hbar} \right)^2 + \frac{N(N-1)(N-2)}{3!} \left(\frac{iJ_z\phi}{N\hbar} \right)^3 + \dots \right] \\ &= \exp \left(-\frac{i}{\hbar} J_z \phi \right). \end{aligned} \quad (1.50)$$

Angular momentum can thus be considered as the generator of rotations.

Rotation properties

- **Identity.** $\exists I$ such that $IU = UI = U$.
- **Closure.** $U_1 U_2$ is also a rotation U_3 .
- **Inverse.** \exists an inverse such that $UU^{-1} = I$.
- **Associativity.** $(U_1 U_2) U_3 = U_1 (U_2 U_3)$.

Commutation properties

Recall in PH3101 and 3D rotations in classical physics,⁴ $R_x(\epsilon)R_y(\epsilon) - R_y(\epsilon)R_x(\epsilon) = R_z(\epsilon^2) - \mathbb{I}$. In analogy with the classical case, we can write the commutation for the infinitesimal rotations:

$$\begin{aligned} U_x(\epsilon)U_y(\epsilon) - U_y(\epsilon)U_x(\epsilon) &= \left(\mathbb{I} - i \frac{J_x}{\hbar} \epsilon - \frac{J_x^2}{2\hbar^2} \epsilon^2 \right) \left(\mathbb{I} - i \frac{J_y}{\hbar} \epsilon - \frac{J_y^2}{2\hbar^2} \epsilon^2 \right) - \left(\mathbb{I} - i \frac{J_y}{\hbar} \epsilon - \frac{J_y^2}{2\hbar^2} \epsilon^2 \right) \left(\mathbb{I} - i \frac{J_x}{\hbar} \epsilon - \frac{J_x^2}{2\hbar^2} \epsilon^2 \right) \\ &= -\frac{1}{\hbar^2} (J_x J_y - J_y J_x) \epsilon^2 + \mathcal{O}(\epsilon^3), \end{aligned} \quad (1.51)$$

and equate this to $U_z(\epsilon^2) - \mathbb{I} = -\frac{i}{\hbar} J_z \epsilon^2$. With this analogy we justify the definition of angular momentum operators as operators that generate the rotations and obey the commutation relationships:

$$[J_i, J_j] = i\hbar \epsilon_{ijk} J_k, \quad (1.52)$$

where ϵ_{ijk} is the completely antisymmetric or Levi-Civita tensor⁵ and we assume a sum over repeated indices.

1.3.2 Spin 1/2 and Pauli Operators

The lowest dimension in which the commutation relationships above hold is 2. The spin angular momentum, or spin \vec{S} , for a two-level system is represented by the Pauli operators $\sigma_{x,y,z}$,

$$S_x = \frac{\hbar}{2} \sigma_x = \frac{\hbar}{2} (|0\rangle\langle 1| + |1\rangle\langle 0|), \quad (1.53)$$

$$S_y = \frac{\hbar}{2} \sigma_y = \frac{i\hbar}{2} (|0\rangle\langle 1| - |1\rangle\langle 0|), \quad (1.54)$$

$$S_z = \frac{\hbar}{2} \sigma_z = \frac{\hbar}{2} (|0\rangle\langle 0| - |1\rangle\langle 1|). \quad (1.55)$$

Here, $|0\rangle, |1\rangle$ are eigenstates of S_z with eigenvalues $\pm\hbar/2$.

■ **Example 1.10** Write the Pauli operators as matrices in the $\{|0\rangle, |1\rangle\}$ basis. ■

⁴See, e.g. Sakurai, Chapter 3.1 for details.

⁵See, e.g. Wikipedia (Levi-Civita symbol > three dimensions) https://en.wikipedia.org/wiki/Levi-Civita_symbol#Three_dimensions

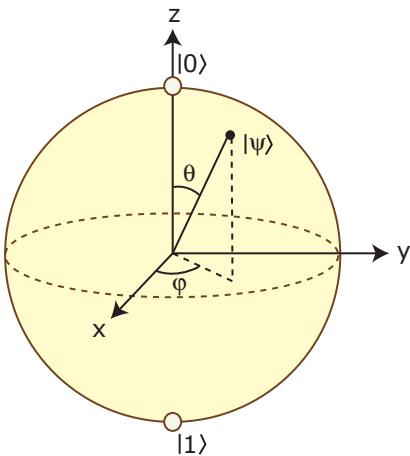


Figure 1.1: **Bloch sphere.** The Bloch sphere is of unit radius, and a pure state is represented by a Bloch vector pointing from the centre to the surface. Logical states $|0\rangle / |1\rangle$ are on the North/South poles. Polar angle θ and azimuthal (phase) angle ϕ are as given in Eq. (1.65).

Pauli Operators

The Pauli operators have the following properties:

$$\sigma_i^2 = \mathbb{I} \quad (1.56)$$

$$\text{anti-commutation relation: } \{\sigma_i, \sigma_j\} \equiv \sigma_i \sigma_j + \sigma_j \sigma_i = 2\delta_{ij}\mathbb{I} \quad (1.57)$$

$$\text{commutation relation (Eq. (1.52)): } [\sigma_i, \sigma_j] \equiv \sigma_i \sigma_j - \sigma_j \sigma_i = 2i\epsilon_{ijk}\sigma_k \quad (1.58)$$

$$\text{Hermitian: } \sigma_i^\dagger = \sigma_i \quad (1.59)$$

$$\text{unitary: } \sigma_i^\dagger = \sigma_i^{-1} \quad (1.60)$$

$$\text{traceless: } \text{Tr}(\sigma_i) = 0 \quad (1.61)$$

$$\text{determinant: } \text{Det}(\sigma_i) = -1 \quad (1.62)$$

The first three relations can be combined into another form:

$$\text{closure: } \sigma_i \sigma_j = \delta_{ij}\mathbb{I} + i\epsilon_{ijk}\sigma_k \quad (1.63)$$

1.3.3 Two level systems

The basic states of a qubit are usually termed $|0\rangle$ and $|1\rangle$, corresponding to binary bits in classical computing. In the 2-dimensional Hilbert space, they are given a vector representation,

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (1.64)$$

A quantum state can then be written as $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$, where $\alpha, \beta \in \mathbb{C}$, and $|\alpha|^2 + |\beta|^2 = 1$. Since a global phase is not measurable, we can “factor it away” and without loss of generality, rewrite the state as

$$|\psi\rangle = \cos \frac{\theta}{2} |0\rangle + e^{i\phi} \sin \frac{\theta}{2} |1\rangle. \quad (1.65)$$

This has a nice geometrical representation given by the Bloch sphere in Fig. 1.1. Describing a qubit state via the two angles θ and ϕ leads to a simple geometrical picture for the space occupied by this system. The angles define a point on a sphere of radius 1. A state represented by a point on the surface is called a pure state. Any point on the surface of the sphere can be reached from another point by a unitary transformation. In quantum computing terminology, this is called a single-qubit rotation. We will also be interested in the points inside the sphere (called mixed states) in the open systems part of the course later.

1.3.4 Rotations on the Bloch sphere

■ **Example 1.11 Discrete rotations.** What is the action of the Pauli operators on the qubit state $|\psi\rangle = a|0\rangle + b|1\rangle$? ■

■ **Example 1.12 Continuous rotations.** Calculate the time-evolution of a qubit when it starts out in the initial state,

$$|\psi(0)\rangle = \cos \frac{\theta}{2} |0\rangle + e^{i\phi} \sin \frac{\theta}{2} |1\rangle$$

when subjected to the following Hamiltonians:

- (i) $H = \hbar \frac{\omega}{2} \sigma_z$, for initial angles $\theta = \pi/2$ and $\phi = 0$.
- (ii) $H = \hbar \lambda \sigma_x$, for initial angle $\theta = 0$ and $\phi = 0$.
- (iii) $H = \hbar \lambda \sigma_y$, for initial angle $\theta = 0$ and $\phi = 0$.

Note that we can use the results⁶ from Eqs. (1.25) and (1.28) to do the matrix exponentiation, or use the definition in Eq. (1.21) applied to the exponentiation function,

$$\exp(A) = \sum_{k=0}^{\infty} \frac{1}{k!} A^k, \quad (1.66)$$

where A can be an operator or a square, real or complex matrix, and A^0 is defined to be the identity matrix. ■

Since any operator on a two-level space can be written in terms of the Pauli operators, if we know the properties of the Pauli operators under exponentiation, we can derive a general formula for the unitary evolution of a qubit state. First, we note that

$$\begin{aligned} (\vec{\sigma} \cdot \hat{n})^2 &= (\sigma_x n_x + \sigma_y n_y + \sigma_z n_z)^2 \\ &= \sigma_x^2 n_x^2 + n_x n_y (\underbrace{\sigma_x \sigma_y + \sigma_y \sigma_x}_{\text{cross terms vanish by Eq. (1.57)}}) + \dots \\ &= n_x^2 \mathbb{I} + n_y^2 \mathbb{I} + n_z^2 \mathbb{I} \quad (\text{using Eq. (1.56)}) \\ &= \mathbb{I}, \quad (\text{since } \hat{n} \text{ is a unit vector}) \end{aligned} \quad (1.67)$$

and

$$(\vec{\sigma} \cdot \hat{n})^3 = (\vec{\sigma} \cdot \hat{n})^2 (\vec{\sigma} \cdot \hat{n}) = \mathbb{I} (\vec{\sigma} \cdot \hat{n}) = (\vec{\sigma} \cdot \hat{n}). \quad (1.68)$$

Next, we perform a Taylor series expansion of the exponential and separate even and odd powers to obtain

$$\begin{aligned} \exp \{-i\theta \vec{\sigma} \cdot \hat{n}\} &= \sum_{k=0}^{\infty} \frac{(-i\theta \vec{\sigma} \cdot \hat{n})^k}{k!} \\ &= \left(\sum_{k \text{ even}} \frac{(-i\theta \vec{\sigma} \cdot \hat{n})^k}{k!} \right) + \left(\sum_{k \text{ odd}} \frac{(-i\theta \vec{\sigma} \cdot \hat{n})^k}{k!} \right) \\ &= \underbrace{\mathbb{I} \left(1 - \frac{\theta^2}{2!} + \frac{\theta^4}{4!} - \dots \right)}_{=\cos \theta} - i \underbrace{\vec{\sigma} \cdot \hat{n} \left(\frac{\theta}{1!} - \frac{\theta^3}{3!} + \frac{\theta^5}{5!} - \dots \right)}_{=\sin \theta}. \end{aligned} \quad (1.69)$$

Therefore, we have a useful relation,

$$e^{-i\theta \vec{\sigma} \cdot \hat{n}} = \cos \theta \mathbb{I} - i \sin \theta \vec{\sigma} \cdot \hat{n} \quad (1.70)$$

⁶ $\exp(\sigma_z) = \exp \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} e^1 & 0 \\ 0 & e^{-1} \end{pmatrix}$ and $\sigma_x = U_1 \sigma_z U_1^\dagger$, where $U_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$ and $\sigma_y = U_2 \sigma_z U_2^\dagger$, where $U_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}$.

This relation is very useful for computing time-evolution of qubit states under a general Hamiltonian, $H = \hbar(\omega_x\sigma_x + \omega_y\sigma_y + \omega_z\sigma_z)$. Taking $\vec{\omega} = (\omega_x, \omega_y, \omega_z)^T$, the time-evolution can be expressed as

$$\begin{aligned} U(t, 0) &\equiv U(t) = \exp\{-iHt/\hbar\} \\ &= \exp\{-it\vec{\omega} \cdot \vec{\sigma}\} \\ &= \exp\{-i(\omega t)\hat{\omega} \cdot \vec{\sigma}\}, \end{aligned} \quad (1.71)$$

where $\omega = \sqrt{\omega_x^2 + \omega_y^2 + \omega_z^2}$ and $\hat{\omega} = \left(\frac{\omega_x}{\omega}, \frac{\omega_y}{\omega}, \frac{\omega_z}{\omega}\right)^T$. Defining $\theta = \omega t$ and using Eq. (1.69), we get in matrix form,

$$\begin{aligned} U(t) &= \exp\{-it\vec{\omega} \cdot \vec{\sigma}\} = \cos(\omega t) \mathbb{I} - i \sin(\omega t) \vec{\sigma} \cdot \hat{\omega} \\ &= \begin{pmatrix} \cos(\omega t) - i \frac{\omega_z}{\omega} \sin(\omega t) & (-i \frac{\omega_x}{\omega} - \frac{\omega_y}{\omega}) \sin(\omega t) \\ (-i \frac{\omega_x}{\omega} + \frac{\omega_y}{\omega}) \sin(\omega t) & \cos(\omega t) + i \frac{\omega_x}{\omega} \sin(\omega t) \end{pmatrix}. \end{aligned} \quad (1.72)$$

1.4 Three Pictures of Quantum Mechanics

There are three equivalent dynamical pictures (or representations) to mathematically formulate the dynamics of a quantum system, the Schrödinger, Heisenberg and interaction (or Dirac) pictures.

	Schrödinger picture	Interaction picture	Heisenberg picture
State ket	Evolution determined by H	Evolution determined by V^I	No change
Observable	No change	Evolution determined by H_0	Evolution determined by H

1.4.1 Schrödinger Picture

Until now we described the dynamics of quantum mechanics by looking at the time evolution of the state vectors as $|\psi(t)\rangle = U(t)|\psi(0)\rangle$, where the state vector obeys the Schrödinger equation $i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle$.

For a time-independent Hamiltonian, the spectral decomposition of the Hamiltonian is defined in terms of its energy eigenvalues ϵ_k and eigenstates $|k\rangle$: i.e. $H = \sum_k \epsilon_k |k\rangle \langle k|$. The unitary time-evolution operator is then given by

$$U(t) = \exp\left\{-\frac{i}{\hbar}Ht\right\} = \exp\left\{-\frac{i}{\hbar}\sum_k \epsilon_k t |k\rangle \langle k|\right\} = \sum_k e^{-i\varphi_k(t)} |k\rangle \langle k|, \quad (1.73)$$

where the eigen-phases are defined as $\varphi_k(t) \equiv \omega_k t$, with $\hbar\omega_k \equiv \epsilon_k$. For a time-independent Hamiltonian, we have $U^\dagger(t) = U(-t)$, which implies that the system dynamics is time-reversible.

■ **Example 1.13** Using Eq. (1.73), find (i) the time-evolution of a system initially in state $|\psi\rangle = \sum_k c_k |k\rangle$, where $|k\rangle$ are energy eigenkets, and (ii) the time-evolution of the expectation value of an observable $\langle A(t)\rangle$.

This perspective to quantum dynamics is called the Schrödinger picture, where states evolve with time while operators are fixed. ■

1.4.2 Heisenberg Picture

From Example (1.13), one can define the time-evolved version of the observable, $A(t) = U^\dagger A U$, from which we can obtain expectation values while considering states that are fixed in time. This is the Heisenberg picture.

To be precise, observables in the Heisenberg picture are defined as

$$A^H(t) = U^\dagger(t) A^S U(t), \quad \text{where } A^H(0) = A^S \quad \text{and } U = \exp\left\{-\frac{i}{\hbar}Ht\right\}. \quad (1.74)$$

That is, observables evolve with time in the Heisenberg picture.

The states in the two pictures coincide at time $t = 0$,

$$|\psi\rangle^H = |\psi(0)\rangle^S, \quad (1.75)$$

and states in the Heisenberg picture remain independent of time. The equation of motion of the Heisenberg picture for time-independent Hamiltonian is given by

$$\begin{aligned} \frac{dA^H}{dt} &= \frac{d(U^\dagger A^S U)}{dt} = \underbrace{\frac{i}{\hbar} H U^\dagger}_{\text{note } U, U^\dagger, H \text{ commute for time-indep. } H} A^S U + U^\dagger A^S \underbrace{\frac{\partial U}{\partial t}}_{-\frac{i}{\hbar} H U} + U^\dagger \underbrace{\frac{\partial A^S}{\partial t} U}_{\equiv \left(\frac{\partial A^S}{\partial t}\right)^H} \\ &= \underbrace{\left(\frac{i}{\hbar} U^\dagger H\right) A^S U + U^\dagger A^S \left(-\frac{i}{\hbar} H U\right)}_{\text{(inserting } \mathbb{I}=UU^\dagger\text{)}} + \left(\frac{\partial A^S}{\partial t}\right)^H \\ &= \frac{i}{\hbar} \underbrace{(U^\dagger H U U^\dagger A^S U - U^\dagger A^S U U^\dagger H U)}_{\text{(defining } H^H=U^\dagger H U\text{)}} + \left(\frac{\partial A^S}{\partial t}\right)^H \\ &\therefore \frac{dA^H}{dt} = -\frac{i}{\hbar} [A^H, H^H] + \left(\frac{\partial A^S}{\partial t}\right)^H. \end{aligned} \quad (1.76)$$

Since for time-independent H , the unitary operators U and U^\dagger always commute with H , so we always have $H^H = H$. Therefore,

Heisenberg equation of motion

$$\frac{dA^H}{dt} = -\frac{i}{\hbar} [A^H, H] + \left(\frac{\partial A^S}{\partial t}\right)^H. \quad (1.77)$$

1.4.3 Interaction Picture

There is another perspective, called the interaction (or Dirac) picture, which was formulated by Dirac to solve time-dependent perturbation problems. This is particularly useful when the Hamiltonian comprises a solvable, time-independent term H_0 and a perturbation term $V(t)$, which may be time-dependent.

$$H = H_0 + V(t). \quad (1.78)$$

Typically, the dynamics due to H_0 are known and perhaps uninteresting, and we are only interested in the dynamics generated by the perturbation $V(t)$. The state and operators in the interaction picture are given by

$$|\psi\rangle^I = U_0^\dagger(t) |\psi\rangle^S = e^{iH_0 t/\hbar} |\psi\rangle^S \implies |\psi\rangle^S = U_0(t) |\psi\rangle^I, \quad (1.79)$$

$$A^I = U_0^\dagger(t) A^S U_0(t) \implies V^I(t) = U_0^\dagger(t) V(t) U_0(t), \quad (1.80)$$

where $U_0(t) \equiv e^{-iH_0 t/\hbar}$. Similar to the Heisenberg picture, the state vectors coincide at $t = 0$, i.e. $|\psi(0)\rangle^I = |\psi(0)\rangle^S$ and $U_0(0) = \mathbb{I}$. The equation of motion in the interaction picture is therefore,

$$\begin{aligned} i\hbar \frac{\partial |\psi\rangle^I}{\partial t} &= i\hbar \frac{\partial}{\partial t} (U_0^\dagger(t) |\psi\rangle^S) \\ &= i\hbar \frac{\partial U_0^\dagger}{\partial t} |\psi\rangle^S + i\hbar U_0^\dagger \frac{\partial |\psi\rangle^S}{\partial t} \\ &= -U_0^\dagger H_0 |\psi\rangle^S + U_0^\dagger (H_0 + V) |\psi\rangle^S \\ &= U_0^\dagger V U_0 |\psi\rangle^I. \end{aligned} \quad (1.81)$$

Therefore,

Interaction picture equation of motion (state vector)

$$i\hbar \frac{\partial |\psi\rangle^I}{\partial t} = V^I |\psi\rangle^I. \quad (1.82)$$

That is, the interaction picture state vector $|\psi\rangle^I$ evolves according to the dynamics generated by the perturbation V^I only. However, in contrast to the usual Schrödinger picture, even the observables in the interaction picture evolve in time. From their definition $A^I = U_0^\dagger A^S U_0$, we have the differential equation,

Interaction picture equation of motion (observables)

$$\frac{dA^I}{dt} = -\frac{i}{\hbar} [A^I, H_0] + \left(\frac{\partial A^S}{\partial t} \right)^I. \quad (1.83)$$

This is similar to the Heisenberg picture. The interaction picture is thus an intermediate picture between the other two pictures.

1.4.4 Baker-Campbell-Hausdorff (BCH) Formula

Typically, one makes use of the interaction picture when H_0 is time-independent and its eigen-decomposition is known, and $V(t)$ is a time-dependent perturbation. The time-dependence makes evolution complicated, and $V(t)$ may not commute with itself at different points in time. In general,

$$e^{A+B} \neq e^A e^B \text{ if } [A, B] \neq 0. \text{ Conversely, } [A, B] = 0 \implies e^{A+B} = e^A e^B. \quad (1.84)$$

For example, if $V(t)$ does not commute between time intervals $[0, t_1]$ and $[t_1, t]$, then even though the time-evolution operator can be written as

$$U(t, t_0) = U(t, t_1)U(t_1, t_0) = \exp \left\{ -\frac{i}{\hbar} \int_{t_1}^t (H_0 + V(t')) dt' \right\} \exp \left\{ -\frac{i}{\hbar} \int_0^{t_1} (H_0 + V(t')) dt' \right\}, \quad (1.85)$$

it cannot be given an explicit solution in terms of an integral,

$$U(t, 0) \neq \exp \left\{ -\frac{i}{\hbar} \int_{t_1}^t (H_0 + V(t')) dt' - \frac{i}{\hbar} \int_0^{t_1} (H_0 + V(t')) dt' \right\}. \quad (1.86)$$

The Baker-Campbell-Hausdorff (BCH) formula, and especially the related Baker-Hausdorff lemma, will be useful when computing the unitary transformations. We state these without proof here.

BCH formula

If we want C such that $e^C = e^A e^B$, then

$$C = A + B + \frac{1}{2}[A, B] + \frac{1}{12}([A, [A, B]] - [B, [A, B]]) - \frac{1}{24}[B, [A, [A, B]]] \dots \quad (1.87)$$

An additional formula that comes out of this, which is especially useful in quantum mechanics is given by the Baker-Hausdorff lemma:

$$e^{sA} B e^{-sA} = B + s[A, B] + \frac{s^2}{2!}[A, [A, B]] + \frac{s^3}{3!}[A, [A, [A, B]]] + \dots \quad (1.88)$$

When $s = it/\hbar$ and $A = H_0$, the second formula becomes helpful in finding the time evolution of an operator B in the interaction picture, $e^{itH_0/\hbar} B e^{-itH_0/\hbar}$. When the commutator $[H_0, V]$ and its higher order nested commutators are evaluated, and if a closed form expression can be

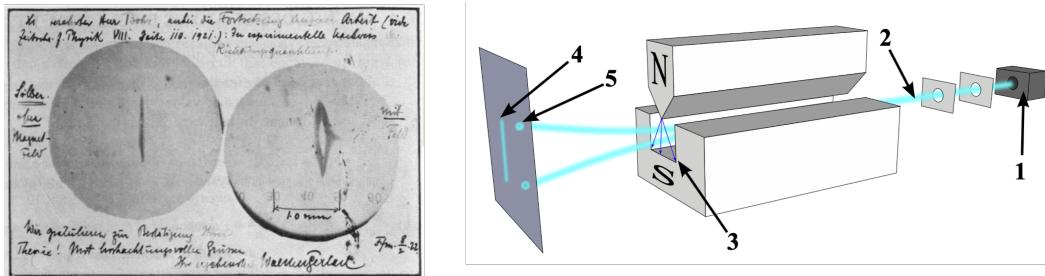


Figure 1.2: Stern Gerlach Experiment. Left (from Physics Today): Gerlach's postcard, dated 8 February 1922, to Niels Bohr. It shows a photograph of the beam splitting, with the message, in translation: "Attached [is] the experimental proof of directional quantization. We congratulate [you] on the confirmation of your theory." Right (from Wikipedia: Stern-Gerlach Experiment): Silver atoms travelling through an inhomogeneous magnetic field, and being deflected up or down depending on their spin; (1) furnace, (2) beam of silver atoms, (3) inhomogeneous magnetic field, (4) classically expected result, (5) observed result.

found for the infinite series (which may not be possible in general), exact solutions can then be found.

■ **Example 1.14 Heisenberg picture.** The Hamiltonian of a simple harmonic oscillator, in terms of the creation \hat{a}^\dagger and annihilation \hat{a} operators, is

$$H = \hbar\omega(\hat{a}^\dagger\hat{a} + \frac{1}{2}), \quad (1.89)$$

where $[\hat{a}, \hat{a}^\dagger] = 1$ and the number states $|n\rangle$ are orthonormal eigenstates of the number operator $\hat{n} \equiv \hat{a}^\dagger\hat{a}$, such that $\hat{n}|n\rangle = n|n\rangle$, $n = 0, 1, 2, \dots$. The action of the creation and annihilation operators on the number states are

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle, \text{ with } \hat{a}|0\rangle = 0; \quad \hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle. \quad (1.90)$$

Determine the Heisenberg equations of motion for the creation and annihilation operators and solve for $\hat{a}(t)$ and $\hat{a}^\dagger(t)$ in the Heisenberg picture. ■

1.5 Quantum Phenomena Do Not Occur in a Hilbert Space

Finally, after much mathematical formalism, we come to the subject of the quote by Asher Peres at the start of this chapter.

Most people would believe that an objective reality exists, and the purpose of science is to uncover and understand it. We acquire knowledge about this reality through the methods of science, which include observation, theory and measurement. Quantum phenomena, however, is incompatible with the notion that measurements uncover some unknown but preexisting reality. As a quintessential example, consider the historic Stern-Gerlach experiment, given a more modern interpretation.

1.5.1 Stern-Gerlach Experiment

In this experiment⁷, Otto Stern and Walther Gerlach measured the deflection of a beam of neutral silver atoms by an inhomogeneous magnetic field. The purpose was to determine the magnetic moment of the atoms from the deflection. Today, we know that there are 47 electrons in a silver atom, of which 46 can be visualized as a spherically symmetric cloud with no net angular momentum. The angular momentum of a silver atom is solely due to the 47-th electron, which, in the $5s$ shell has no orbital angular momentum. Therefore the angular momentum of a

⁷If you wish to listen to Richard Feynman give this lecture, go to https://www.feynmanlectures.caltech.edu/III_05.html and click on the "Original Lecture Recording" icon on the right panel. Remember to turn on the sound!

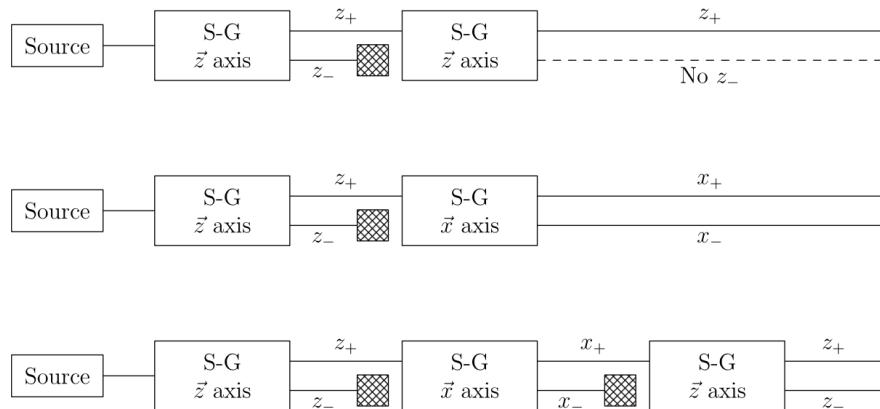


Figure 1.3: **Sequential Stern Gerlach Experiment.** Figure from Wikipedia.

silver atom is solely due to the intrinsic angular momentum (which is also called spin angular momentum) of the 47-th electron. Classical theory would give the Hamiltonian of the atom as

$$H = \frac{\vec{p}^2}{2m} - \vec{\mu} \cdot \vec{B}, \quad (1.91)$$

where \vec{p} is the momentum, \vec{B} the external magnetic field and $\vec{\mu}$ the intrinsic magnetic moment.

Classically, $\vec{\mu}$ is a vector that points in some direction in space, with a continuous distribution of its orientation. If one wanted to know what direction it pointed in, one could measure the x , y and z -components, $\mu_{x,y,z}$.

If the magnetic moment is due to some internal rotational motion around a symmetry axis, we have $\vec{\mu} \propto \vec{S}$, where \vec{S} is the angular momentum around the centre of mass of the atom. If the inhomogeneity of the field is predominantly in the z -direction, the magnetic force experienced by the atom would be

$$F_z = -\frac{\partial}{\partial z}(-\vec{\mu} \cdot \vec{B}) \approx \mu_z \frac{\partial B_z}{\partial z}. \quad (1.92)$$

Therefore, the beam is expected to get deflected (split) according to the values of μ_z . A sample of silver was heated in the oven and allowed to be ejected through an opening (preparation). If the silver atoms were randomly oriented, then there is no preferential orientation of $\vec{\mu}$, and we would expect all values of $-|\mu| \leq \mu_z \leq +|\mu|$ and a **continuous distribution of deflected trajectories** in the z -direction. Instead, what was observed in the experiment was that the **silver atoms were detected at two spots** corresponding to $\pm|\mu|$, an observation theorized in early quantum theory as “space quantization”. It took several more years before the angular momentum states of the silver atom was understood, and the Stern-Gerlach experiment recognized as experimental confirmation of the spin of the electron.⁸ This quantization of spin angular momentum into two discrete components, $S_z = \pm \frac{\hbar}{2}$, is the first important feature we can deduce from the Stern-Gerlach experiment.⁹

1.5.2 Sequential Stern-Gerlach Experiments

Now consider a sequential Stern-Gerlach experiment, as shown in Fig. 1.3, when the atomic beam is subject to two or more SG apparatus in sequence. In the top figure, the atomic beam is split into $z+$ and $z-$ components, and the latter is blocked. The remaining $z+$ beam is subject to a second SG- \vec{z} apparatus. This time, there is only one beam coming out of the second apparatus – the $z+$ beam – which is not a surprise.

In the middle figure, the second apparatus is now a SG- \vec{x} apparatus. The interesting outcome is that two components emerge from the second apparatus, an $x+$ and an $x-$ component, with equal intensities. How can we explain this? Does it mean that 50% of atoms in the $z+$

⁸Electron spin was discovered by George Uhlenbeck and Samuel Goudsmit from the anomalous Zeeman effect.

⁹It was called *space quantization* historically. This term is now defunct.

beam coming out of the first apparatus ($\text{SG-}\vec{z}$) are made up of atoms with pairs of *pre-existing* properties $(x+, z+)$ and the other 50% with $(x-, z+)$? This line of reasoning, based on classical notions and everyday experience, runs into difficulties in the next step.

We now consider a third step, in the bottom figure, where an $\text{SG-}\vec{z}$ apparatus is added. This time, it is observed experimentally, that two components emerge from this third apparatus, i.e. the emerging beams have $z+$ and $z-$ components. This is a complete surprise because after the atoms emerged from the first apparatus, the $z-$ component was completely blocked. How is it possible that the $z-$ component, which we thought had been eliminated earlier, reappears?

1.5.3 Quantum-mechanical treatment of Stern-Gerlach experiment

If we accept that the scope of quantum mechanics is, according to Asher Peres,

in a strict sense, . . . a set of rules allowing the computation of probabilities for the outcomes of tests which follow specified preparations...

then the standard quantum-mechanical treatment of the Stern-Gerlach experiment can be successfully used to compute the probabilities of observing the components that emerge after a measurement or test, given a preparation procedure.

In the quantum-mechanical treatment of the Stern-Gerlach experiment, the spin states of the electron can be described using two orthonormal basis vectors

$$|z;+\rangle \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |z;-\rangle \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad \langle z;+|z;-\rangle = 0, \quad \langle z;+|z;+ \rangle = \langle z;-|z;-\rangle = 1. \quad (1.93)$$

In addition, the $|z;\pm\rangle$ states are eigenstates of the S_z operator, which can be written in the eigenbasis as

$$S_z |z;\pm\rangle = \pm \frac{\hbar}{2} |z;\pm\rangle, \quad S_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (1.94)$$

But there is nothing special about the z -axis. We could have started with a SG apparatus measuring in the x , y or even an arbitrary n axis, and been led to

$$S_x |x;\pm\rangle = \pm \frac{\hbar}{2} |x;\pm\rangle, \quad S_y |y;\pm\rangle = \pm \frac{\hbar}{2} |y;\pm\rangle, \quad S_n |n;\pm\rangle = \pm \frac{\hbar}{2} |n;\pm\rangle. \quad (1.95)$$

In the $|z;\pm\rangle$ basis,

$$S_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad S_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad (1.96)$$

$$\begin{aligned} S_n &= \vec{S} \cdot \hat{n} \\ &= n_x S_x + n_y S_y + n_z S_z \\ &= \sin \theta \cos \phi S_x + \sin \theta \sin \phi S_y + \cos \theta S_z \\ &= \frac{\hbar}{2} \begin{pmatrix} \cos \theta & \sin \theta e^{-i\phi} \\ \sin \theta e^{i\phi} & -\cos \theta \end{pmatrix}. \end{aligned} \quad (1.97)$$

with respective eigenstates

$$|x;\pm\rangle = \frac{1}{\sqrt{2}} (|z;+\rangle \pm |z;-\rangle), \quad (1.98)$$

$$|y;\pm\rangle = \frac{1}{\sqrt{2}} (|z;+\rangle \pm i |z;-\rangle), \quad (1.99)$$

$$|n;\pm\rangle = \cos(\frac{\theta}{2}) |z;+\rangle \pm \sin(\frac{\theta}{2}) e^{i\phi} |z;-\rangle. \quad (1.100)$$

In standard quantum-mechanical language, having prepared a $|z;+\rangle$ state, one has a *superposition* of states, $|z;+\rangle = (|x;+\rangle + |x;-\rangle)/\sqrt{2}$, and upon measurement in the x -axis, the state is forced to “collapse” into either $|x;+\rangle$ or $|x;-\rangle$. Finally, when one of these beams, $|x;+\rangle$, is measured in the z -axis, it is found that the prior measurement in the x -axis had “erased” all information about its z -orientation. Or, in other words, observables S_x and S_z are incompatible.

The Stern-Gerlach experiment contains the quintessential conceptual ingredients of the quantum mechanical picture of physical reality. They may be summarized as follows.

Quantum Concepts

1. **Quantization.** This quantization of spin angular momentum into two discrete components, $S_n = \pm \frac{\hbar}{2}$, in some specified orientation given by an axis \hat{n} .
2. **Incompatible observables.** It is not possible to obtain information about any two orthogonal components of spin angular momentum simultaneously.
3. **Fundamental randomness.** Given a spin prepared in some component, say $z+$, when measuring in another axis, say x , it is impossible to determine which outcome $x+$ or $x-$, will emerge.

While point 1 may not be unfamiliar to early quantum physicists who also discovered the discretized orbits of the atom, point 2 is a more radical departure from classical concepts. It implies that the question “what is the orientation of the spin angular momentum of the atom, $\vec{\mu}$ ” cannot be answered, and has no meaning. A legitimate question, which can be answered experimentally by a device such as that described in the preceding section, is whether or not an atom has a *specified* component of $\vec{\mu}$.

Furthermore, if an experimenter, Alice, prepares a sequence of single particle spins with specified components, and sent them on to another experimenter, Bob, without disclosing the prepared components, there is no instrument whatsoever by which Bob could sort each of these single particles spin into components that agree with the record of Alice’s preparation. *It is fundamentally impossible to measure the spin of a single particle of unknown origin.* The notion of “physical reality” thus acquires new meaning with quantum phenomena, different from its meaning in classical physics. And it requires a new language - quantum mechanics - for dealing with quantum phenomena.

Quantum mechanics, with the principle of superposition, is able to compute the correct probabilities in the Stern-Gerlach experiment (and more). This principle of superposition is fundamental to quantum mechanics, yet when we try to go beyond computing probabilities (the strictly limited scope of quantum mechanics according to Peres) to conceive of the meaning of a superposition of states, we fail. According to Paul A. M. Dirac,

The general principle of superposition of quantum mechanics applies to the states ... of any one dynamical system. It requires us to assume that between these states there exist peculiar relationships such that whenever the system is definitely in one state we can consider it as being partly in each of two or more other states. The original state must be regarded as the result of a kind of superposition of the two or more new states, in a way that cannot be conceived on classical ideas.

If we accept that a measurement is not a passive acquisition of knowledge, but an active process involving the interaction of a macroscopic measurement apparatus and the microscopic system, and that experimental outcomes must be *interpreted* through the construct of a theoretical model, then according to Kemble¹⁰,

we have no satisfactory reason for ascribing objective existence to physical quantities as distinguished from the numbers obtained when we make the measurements which we correlate with them. There is no real reason for supposing that a particle has at every moment a definite, but unknown, position which may be revealed by a measurement of the right kind, or a definite momentum which can be revealed by a different measurement. On the contrary, we get into a maze of contradictions as soon as we inject into quantum mechanics such concepts carried over from the language and philosophy of our ancestors... It would be more exact if we spoke of “making measurements” of this, that, or the other type instead of saying that we measure this, that, or the other “physical quantity.”

¹⁰E. C. Kemble, The Fundamental Principles of Quantum Mechanics, McGraw-Hill, New York (1937) [reprinted by Dover] pp. 243-244.

Finally, when probed as to what was the underlying reality, i.e. the “quantum world”, that mirrored or corresponded to the mathematical formalism, Niels Bohr famously said, with clear anti-realist overtones,¹¹

There is no quantum world. There is only an abstract quantum physical description. It is wrong to think that the task of physics is to find out how nature is. Physics concerns what we can say about Nature.

1.6 References

1. **Linear Algebra:** Nielsen and Chuang, Chap 2.1, or Sakurai, Chap 1.
2. **Postulates:** Nielsen and Chuang, Chap 2.2.
3. **Angular Momentum:** Sakurai, Chap 3.1 and 3.2.
4. **Stern-Gerlach Experiment:** Sakurai, Chap 1.1.
5. **Three pictures:** Sakurai, Chap 2.2 and 5.5

1.7 Discussion Set

Part I: Concepts

Problem 1.1 Global phase.

Consider the two states given below, which differ by a global phase $e^{-i\phi/2}$.

$$|\psi\rangle = \cos \frac{\theta}{2} |0\rangle + e^{i\phi} \sin \frac{\theta}{2} |1\rangle, \quad (1.101)$$

$$|\varphi\rangle = e^{-i\phi/2} \cos \frac{\theta}{2} |0\rangle + e^{i\phi/2} \sin \frac{\theta}{2} |1\rangle. \quad (1.102)$$

Show that a global phase factor does not change measurement outcomes and measurement statistics by considering a general observable \hat{A} with eigenvectors $|a_i\rangle = \alpha_i |0\rangle + \beta_i |1\rangle$.

Problem 1.2 “Illegal” Hamiltonian.

Suppose a Hamiltonian was mistakenly written as

$$H = H_{11} |1\rangle \langle 1| + H_{22} |2\rangle \langle 2| + H_{12} |1\rangle \langle 2|. \quad (1.103)$$

What principle is now violated? Illustrate your point by explicitly attempting to solve the most general time-dependent problem using an “illegal” Hamiltonian of this kind. For simplicity, you may assume $H_{11} = H_{22} = 0$.

Problem 1.3 Hadamard gate. The Hadamard gate is a quantum operation on a single qubit governed by the unitary,

$$U_{\text{Hadamard}} = \frac{1}{\sqrt{2}} (\sigma_x + \sigma_z).$$

What is action of the Hadamard gate on each of these states, $|0\rangle, |1\rangle, |+\rangle, |-\rangle$? Deduce its rotation axis on the Bloch sphere.

Problem 1.4 CNOT gate. The control-NOT (CNOT) gate is a quantum operation on two qubits. The logical operation is such that the state of the target qubit (B) is flipped conditionally on the state of the control qubit (A) being 1, and nothing is done when the state of the control qubit is 0. The truth table is analogous to the XOR gate in classical computing, and is given as follows.

input		output	
A (control)	B (target)	A (control)	B (target)
0	0	0	0
0	1	0	1
1	0	1	1
1	1	1	0

¹¹The Philosophy of Niels Bohr, by Aage Petersen. Pp 8-14. Published online: 15 Sep 2015. <https://doi.org/10.1080/00963402.1963.11454520>.

What would be the corresponding unitary operation, written in (i) Dirac notation, and (ii) matrix form?

Part II: Bloch sphere & Bloch vector

Problem 1.5 Bloch vector. A pure state in a two-level system can be represented as a Bloch vector pointing from the centre to the surface of the Bloch sphere? Where would the Bloch vector be pointing to, on the Bloch sphere, corresponding to the following states?

- (i) $|\psi\rangle = |1\rangle$.
- (ii) $|\psi\rangle = (|0\rangle + i|1\rangle)/\sqrt{2}$.
- (iii) $|\psi\rangle = (|1\rangle - |0\rangle)/\sqrt{2}$.
- (iv) $|\psi\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$.
- (v) $|\psi\rangle = i \cos(\pi/8)|0\rangle - \sin(\pi/8)|1\rangle$.

Problem 1.6 Bloch sphere. Verify that a pure state of a two-level system, given by $|\psi\rangle = \cos(\theta/2)|0\rangle + e^{i\phi}\sin(\theta/2)|1\rangle$, can be represented by the Bloch vector and Bloch sphere picture of Fig. 1.1, by calculating the expectation values of the Pauli matrices, $\langle\sigma_x\rangle$, $\langle\sigma_y\rangle$ and $\langle\sigma_z\rangle$. The results should correspond to the geometry associated with the polar and azimuthal angles, θ and ϕ .

Part III: Time evolution of pure states and Three pictures of QM

Problem 1.7 NMR / Spin precession – Schrödinger picture. We consider the semi-classical problem of a spin-1/2 particle (e.g. proton) in a classical magnetic field. Each spin \vec{S} is associated with a magnetic moment $\vec{\mu} = \gamma\vec{S}$, where γ is called the gyromagnetic ratio. The energy of a spin in an external magnetic field is, classically, $-\vec{\mu} \cdot \vec{B}$. Assuming a magnetic field in the z -direction, quantum mechanically, the Hamiltonian is $H = -\gamma BS_z$, where $S_z = \frac{\hbar}{2}\sigma_z$.

Define $|0\rangle \equiv |m_s = +1/2\rangle$, $|1\rangle \equiv |m_s = -1/2\rangle$, and given that the spin is initially in the state $|\psi(0)\rangle = \cos(\theta/2)|0\rangle + \sin(\theta/2)e^{i\phi}|1\rangle$.

In the Schrödinger picture,

- (i) what is the state at a later time $|\psi(t)\rangle$?
- (ii) what is the probability of finding the initial state as a function of time for $\theta = 0, \pi/4, \pi/2$?

Recall: S_z has two eigenstates, $|m_s = \pm 1/2\rangle$ with eigenvalues $\pm \frac{\hbar}{2}$. Also, $\vec{\mu} = -\frac{1}{2}g\mu_B\vec{\sigma}_z$. At the undergraduate level, this is usually derived semi-classically for an electron in circular orbit, by $\vec{\mu} = I\vec{A} = \frac{-e}{2\pi v/r}\pi r^2\hat{A} = \frac{-e}{2m}mv\hat{A} = \frac{-e\vec{L}}{2m}$. Replacing \vec{L} by $\vec{S} = \frac{\hbar}{2}\vec{\sigma}$, we get $\vec{\mu} = -\frac{1}{2}\frac{e\hbar}{2m}\vec{\sigma} = -\mu_B\vec{\sigma}/2$ which is off by a relativistic factor, that we call $g \approx 2$. The Dirac equation provides the correct factor.

Problem 1.8 NMR / Spin precession – Heisenberg picture. Consider the preceding NMR/Spin-precession problem. It can also be solved in the Heisenberg picture. Using the same Hamiltonian and initial state, write the Heisenberg equations of motion for the time-dependent operators $S_x(t)$, $S_y(t)$, and $S_z(t)$. Solve them to obtain $S_{x,y,z}(t)$ as functions of time.

Problem 1.9 Rabi oscillation – Schrödinger picture. An electron confined in a double well potential, or a double quantum dot, may be described by its left and right occupation state, $|L\rangle$ and $|R\rangle$. In the context of quantum computing, this is a charge qubit. The most general state vector may be written as

$$|\alpha\rangle = |R\rangle\langle R|\alpha\rangle + |L\rangle\langle L|\alpha\rangle. \quad (1.104)$$

The electron can tunnel through the potential barrier between the quantum dots, and the Hamiltonian is given by

$$H = \Delta(|L\rangle\langle R| + |R\rangle\langle L|). \quad (1.105)$$

- (i) Find the normalized energy eigenkets, and the corresponding eigenvalues.

- (ii) In the Schrödinger picture, the base kets $|L\rangle, |R\rangle$ are fixed and the state vector evolves with time. Suppose the system is represented by $|\alpha(0)\rangle$ as given above, at $t = 0$. Find the state vector $|\alpha(t)\rangle$ for $t > 0$ by applying the appropriate time-evolution operator $U(t, 0)$ to $|\alpha(0)\rangle$.
- (iii) Apart from applying the time-evolution operator, another way to find the evolution of the state vector is to apply the Schrödinger equation and solve the coupled differential equations. By writing $\langle R|\alpha(t)\rangle = c_R(t)$ and $\langle L|\alpha(t)\rangle = c_L(t)$, derive the coupled differential equations in terms of $c_{L/R}(t)$ and their derivatives, and solve them.
- (iv) Suppose at $t = 0$, the particle is in the right quantum dot with certainty. What is the probability of observing the particle in the left quantum dot as a function of time?
- (v) Suppose there was a typographical error, and the Hamiltonian was wrongly given as $H = \Delta |L\rangle\langle R|$. By explicitly solving the most general time-evolution problem with this Hamiltonian, show that probability conservation is violated.

Problem 1.10 Rabi oscillation – interaction picture. Consider a two-level atom driven by circularly polarized light, with the Hamiltonian

$$\begin{aligned} H(t) &= H_0 + V(t), \\ \text{where } H_0 &= \hbar\omega_0 |e\rangle\langle e|, \\ \text{and } V(t) &= Ae^{-i\omega t} |e\rangle\langle g| + A^* e^{i\omega t} |g\rangle\langle e|. \end{aligned}$$

Here, ground and excited states $|g\rangle, |e\rangle$, are eigenstates of the unperturbed Hamiltonian H_0 . The initial state is $|\psi(0)\rangle^S = |\psi(0)\rangle^I = |g\rangle\langle g|$. By going into the reference frame rotating at ω_0 (i.e. the interaction picture given by $U = e^{-iH_0 t/\hbar}$),

- (i) determine $V^I(t)$, the perturbation in the interaction picture, and
- (ii) determine the state at a later time $|\psi(t)\rangle^I$.
- (iii) Hence, or otherwise, find an expression for the time required for the atom to evolve from $|g\rangle$ to $|e\rangle$, at resonance ($\Omega = \omega$).
- (iv) Plot two graphs of the probability of finding the initial state P_g against time t , one at resonance and one when the perturbation frequency is detuned by Δ , where $\Delta \equiv \omega - \omega_0 \neq 0$. You can assume some numbers for the necessary parameters and make numerical calculations for this part.

