Notes On Quantum Mechanics

Graduation Level

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Àqueles que foram-se embora para Pasárgada e deixaram para trás suas dores

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This text is about a study notebook focused on the subject of Quantum Mechanics. The goal of this notes is to be a good revision reference in the formal aspects of Quantum theory. For completeness, the main reference adopted is the Bellentine's text-book [1], however others important references must be cited like [2, 3].

Quantum Mechanics is a general theory, it is presumed to apply to everything, from subatomic particles to galaxies. But, in this theory, some aspects of the nature was a little bit strange, more precisely: *discreteness*, *diffraction*, and *coherence*.

It was the phenomenon of *discreteness* that gave rise to the name "quantum mechaniccs". Certain dynamical variables were found to take on only a discrete, or *quantized*, set of values (i.e., energy for a particle in a finite potential). The first direct evidence for discrete atomic energy levels was provided by Frank-Hertz (1914). In their experiments, electrons emitted from a hot cathode were accelerated through a gas of Hg vapor by means of adjustable potential applied between the anode and the cathode. Basically, the accelerated electron gain a kinetic energy around the first excitation energy of the gas, in this condition, the electron lose their momentum by inelastic collision by atoms of Hg.

The phenomenon of *diffraction* is characteristic of any wave motion, and is especially familiar for light. Ir occurs because the total wave amplitude is the sum of partial amplitudes that arrive by different path. If this difference arrive in phase, they add constructively (maximum in total intensity); if they arrive out of the phase, they add destructively (minimum in total energy). But, in the context of quantum mechanics, this kinda of observation it is not intrinsically related of "waves" (classical one). In quantum world we can observe the occurrence of diffraction in the reflection of electrons (e.g., wave-particle duality).

Other weird effect in quantum mechanics is the differences aspects of the coherence. In classical optics, coherence refers to the condition of phase stability that is necessary for interference to be observable. In general (quantum mechanics) a coherent tell us about the stability of a quantum superposition like we shall in treatment of Starn Gerlach experiment or in quantum erasure method.

Contents

1 Mathematical Prerequisites

In this chapter we must be convinced that formalism of quantum mechanics "work" and their agree with the experimental description of the reality.

1.1 Linear Vector Space

A linear vector space is a set of elements, called vector, which is closed under addition and multiplication by scalars. That is to say, if ϕ and ψ are vector in a linear space V, then exist $\chi \in V$ such that $\chi = a\phi + b\psi$, where $\{a, b\}$ are arbitrary scalars.

There are two classes of vector of common interest:

1. *Discrete vectors,* which may be represented as columns of complex numbers in a basis;

2. *Spaces of functions* of some type, for example the space of all differentiable functions.

A set of vectors $\{\phi_n\}$ is said to be *linearly independent* (L.I) if no nontrivial linear combination of them sum to zero; that is to say, if the equation $\sum_m c_n\phi_n = 0$ can hold only when $c_n = 0$ for all n.

The maximum number of linearly independent vectors in a space is called the *dimension* of the space. A maximal set of linearly independent vectors is called a basis for the space (and it is not unique).

An *inner product* for a linear vector space associates a scalar (ψ, ϕ) with every ordered pair of vectors. It must satisfy the following:

1. $(\psi, \phi) = a$, where a complex number;
2. $(\phi, \psi) = (\psi, \phi)^*$, Hermitian symmetry;
3. $(\phi, c_1\psi_1 + c_2\psi_2) = c_1(\phi, \psi_1) + c_2(\phi, \psi_2)$, linear in second argument;
4. $(\phi, \phi) \geqslant 0$, with the equality holding $\iff \phi = 0$.

OBS: we can prove that inner products is linear in its second argument, and antilinear in its first.

Theorem 1.1: Orthogonality

orthogonality A set $\mathcal{S} = \{v_i\}_{i=1,\cdots,n}$ (n$\in \mathbb{N}$) of non-null vectors and two-two orthogonal, i.e., $(v_j, v_k) = 0 \implies i \neq k$. Then, all vectors v_i are linearly independent.

Exercise 1.1: Complex numbers

The complex numbers can be consider elements of a linear vector space V, such that $\dim V = 2$?

Exercise 1.2: Linearly independence between functions

Prove that the functions $\{\sin(2x), \sin(x)\}$ are linearly independents.

Exercise 1.3: Orthogonality between functions

Show that the functions from the previous exercise are orthogonal (like theorem 1.1).

Other important aspect of the inner products: their generalizes the concept of angle and length to arbitrary spaces. If the inner product of two vectors is zero, the vectors are said to be orthogonal.

The norm of a vector is defined as $\|\phi\| := (\phi, \phi)^{1/2}$. Some theorems of norms are:

Theorem 1.2: Schawarz's inequality

$|(\psi, \phi)|^2 \leqslant (\psi, \psi)(\phi, \phi)$;

Theorem 1.3: The triangle inequality

$\|\psi + \phi\| \leqslant \|\psi\| + \|\phi\|$.

Exercise 1.4: Schawarz's inequality

Prove the *Schawarz's inequality* (Theorem 1.2).

Exercise 1.5: Triangle inequality

Prove the *Triangle inequality* (Theorem 1.3).

A set of vectors $\{\phi_i\}$ is said to be orthonormal if the vectors are pariwise orthogonal and of unit norm; that is to say, their inner products satisfy $\phi_i, \phi_j) = \delta_{ij}$.

Corresponding to any linear vector space V there exists the dual space of linear functionals on V. A linear functional F assigns a scalar $F(\phi)$ to each vector ϕ, such that:

$$F(a\phi + b\psi) = aF(\phi) + bF(\psi)$$

for any vectors ϕ and ψ, and any scalars a and b. The set of linear functionals may itself be regarded as forming a linear space V' and the sum of two functionals

$$(F_1 + F_2) = F_1(\phi) + F_2(\phi).$$

With this ingredients and the *Riesz Theorem* we say that V' is isomorphic to V

Theorem 1.4: Riesz Theorem

There is one-to-one correspondence between linear functionals F in V' and vectors f in V, such that all linear functionals have the form:

$$F(\phi) = (f, \phi), \tag{1.1}$$

f being fixed vector, and ϕ being arbitrary. Thus, V and V' are essentially isomorphic.

1.2 Dirac's Algebra

In Dirac's notation, the vectors in V is called *ket* vectors, and denoted as $|\cdot\rangle$. Otherwise, the isomorphic vectors in V' are denominated *bra* and denoted as $\langle v|$ or, symbolically

$$\mathcal{L}(v) \equiv \langle v|\cdot\rangle\,. \tag{1.2}$$

Because of the last definition, the linearity in respect to second argument and the hermitian conjugation. For any vectors $|\alpha\rangle = \sum_i c_i |i\rangle$ and $|\beta\rangle$:

$$\begin{aligned}\langle\alpha|\beta\rangle =& (\langle\beta|\alpha\rangle)^* \\ =& \left(\sum_i c_i \langle\beta|i\rangle\right)^* \\ =& \sum_i c_i^* \langle i|\beta\rangle ,\end{aligned}$$

hence,

$$\langle\alpha| \equiv \sum_i c_i^* \langle i| \underset{\longleftrightarrow}{\text{b.c}} |\alpha\rangle . \tag{1.3}$$

1.3 Linear Operators

Operators are maps[1] between two vectorial spaces. An operator A is said *linear operator* if A map any vector ψ into a new other vector ϕ, i.e. $\phi = A\psi$ for all ψ and ϕ any vectors.

The linear operators A and B satisfies

$$A\left(\sum_i \psi_i\right) = \sum_i A(\psi_i) ; \tag{1.4a}$$

$$(A + B)\,\psi = A\psi + B\psi; \tag{1.4b}$$

$$AB(\psi) = A(B(\psi)) . \tag{1.4c}$$

We said that two operators A and B are equal if, and only if, $A\psi = B\psi$ for all ψ.

[1] Or tensors of rank 1, in other point of view.

Example 1.1: Operators as Matrix

In a space n-dimensional with a determined orthonormal discrete basis $\{e_i\}_{i=1,\cdots,n}$. Consider, for example, the equation

$$M|\psi\rangle = \phi,$$

or, in the basis $\{e_i\}$, we have:

$$\begin{aligned}\sum_j \langle e_i|M|e_j\rangle a_j &= \sum_k \langle e_i|e_k\rangle b_k \\ \sum_j M_{ij}a_j &= b_i\end{aligned}$$

where we used $|\psi\rangle = \sum_j a_j |e_j\rangle$, $\phi = \sum_k b_k |e_k\rangle$ with $\{a_i, b_i\} \in \mathbb{C}$.

Example 1.2: Operators in function spaces

Consider a operation:

$$\frac{\partial}{\partial x}x = \mathbb{1} + x\frac{\partial}{\partial x}, \tag{1.5}$$

consists in an operator define in differential function spaces.

Exercise 1.6: Determine an Operator

Determine an operator A which satisfies $A\psi = \phi$, where $\psi \doteq (3,2,1)^\intercal$ and $\phi \doteq (1,0,1)^\intercal$. Is that operator a linear operator?

Exercise 1.7: General Solution For (1.5)

Show that $\psi(x) = \exp(x)$ it is a solution of (1.5), i.e. $\partial_x(x\psi) = a(x)\psi$

Consider the action of an operator A in a vector $|\phi\rangle$:

$$A|\phi\rangle = |\psi\rangle, \tag{1.6}$$

we can compute the *adjoint* as

$$\langle\phi| A^{\dagger} = \langle\psi| \,, \tag{1.7}$$

and because of hermitian symmetry of the inner product

$$\left(\langle\phi|A^{\dagger}|\psi\rangle\right)^{*} = \langle\psi|A|\phi\rangle \,, \tag{1.8}$$

for all ψ and ϕ. Several useful proprieties of the adjoint operator are

$$\begin{aligned}
\left(cA^{\dagger}\right) =& c^{*}A^{\dagger};\\
(A+B)^{\dagger} =& A^{\dagger}+B^{\dagger};\\
(AB)^{\dagger} =& B^{\dagger}A^{\dagger}.
\end{aligned}$$

Note that, the inner product is a scalar, i.e. $\langle\psi|\phi\rangle = a$ for any $\{|\phi\rangle\,, |\psi\rangle \in \mathcal{H}$ and $a \in \mathcal{C}$. In addition to $\langle\psi|\phi\rangle$ we may define in our algebra a *outer product*, this object is an operator

$$|\psi\rangle\langle\phi| \,. \tag{1.9}$$

Due to Hermitian symmetry of conjugation satisfies

$$\left(|\phi\rangle\langle\psi|\right)^{\dagger} = |\psi\rangle\langle\phi| \,. \tag{1.10}$$

Exercise 1.8: Hermitian Conjugation of Outer Product

Prove the equation 1.10.

Exercise 1.9: Trace and basis independence

Prove that the trace of an operator A, $\mathrm{Tr}\, A = \sum_n \langle u_n|A|u_n\rangle$, is independent of the particular orthogonal basis $\{|u_n\rangle\}$ that is chosen for its evaluation.

As we shown, given a basis (e.g., $\{e_i\}_{i\in I}$) and a linear operators (A), A can be represented like a $(\dim I \times \dim I)$-square matrix. Thus, it is possible define the *trace* operation:

$$\mathrm{Tr}\, A := \sum_{i=1}^{\dim I} \langle e_i|A|e_i\rangle\,. \tag{1.11}$$

Specially, the trace operations is invariant under basis changing (see Exercise 1.10). In next chapters how the trace operation becomes one of the most important mathematical propriety to describe a *real* physical state in QM.

Exercise 1.10: Solve the eigenvalue equation

Find the eigenvalues and eigenvectors of the matrix $M = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$

The following theorems are useful in identifying Hermitian operators on a vector space with complex scalars.

Theorem 1.5: Hermitian Operators

If $\langle\psi|A|\psi\rangle = \langle\psi|A|\psi\rangle^*$ for all $|\psi\rangle$, then it follows that $\langle\phi_1|A|\phi_2\rangle = \langle\phi_2|A|\phi_1\rangle^*$ for all $|\phi_j\rangle_{j=1,2}$, and hence $A = A^\dagger$

Theorem 1.6: Eigenvalues and Real Numbers

If A is a Hermitian operator the all of its eigenvalues are real, we must have $\langle\psi|A|\psi\rangle = \langle\psi|A|\psi\rangle^*$

Theorem 1.7: Eigenvectors Orthogonality

Eigenvectors corresponding to distinct eigenvalues of a Hermitian operator must be orthogonal

Exercise 1.11: Self-adjoint Theorems

Prove the previously Theorems (Theorem 1.5, Theorem 1.6, Theorem 1.7)

Properties of complete orthogonal sets

Let be $\mathcal{S} \subset V$ a set of vectors (e.g., $\mathcal{S} = \{\phi_i\} \in V$) such that $V = \text{span}(\mathcal{S})$. In this case we said that $\int$ is *complete*. From the inner product we can determined the components of any vector $|v\rangle \in V$ via $v_i = \langle\phi|v\rangle$. Therefore, the expansion of $|v\rangle$ becomes:

$$|v\rangle = \sum_i \underbrace{(\langle\phi|v\rangle)}_{\equiv v_i} \phi_i. \tag{1.12}$$

Furthermore, the last definition suggests that a certain operator acts on a vector and produces the same vector (identity propriety)[2]. Thus,

$$\sum_i P_i \equiv \sum_i |\phi_i\rangle\langle\phi_i| = \mathbb{1}, \tag{1.13}$$

where P_i define a projector operator (pure mathematical way) and n tell us about of the dimension of the space.

If, for any operator A, $A|\phi_i\rangle = a_i|\phi_i\rangle$ and the eigenvectors form a complete orthogonal set (i.e., satisfies (1.12) and (1.13)), then A can be rewritten as

$$A = \sum_i a_i |\phi_i\rangle\langle\phi_i|. \tag{1.14}$$

It is important to note that any projector operator P_i we have: $P = P^\dagger$ (Hermitian) and $P_i^2 = P_i$ (idempotent).

[2] That is what we call *completeness*.

Exercise 1.12: Proprieties of a Projector Operator

Show that, for any P_i defined as (1.13), P_i is Hermitian and idempotent. Moreover, prove the previously requirements for $P_k := \sum_{i=1}^{d} |\phi_{ki}\rangle\langle\phi_{ki}|$ (a d-degenerate case, where $\{|\phi_{ki}\rangle\}$ forms an orthonormal basis for k-subspace).

1.4 Probability Theory

Together with linear algebra, the probability theory forms a deeper foundation of Quantum Mechanics. In different point of view of Classical Mechanics (CM), the quantum realm treat the nature as a sequence of stochastic process, in other words the Quantum Theory tell about only probabilities and possibilities[3].

To start our discussion of probability theory, let consider the following example:

Example 1.3: Initial Definitions

Let be $P(A|B)$ the probability to find out A under B condition (i.e., $P(A|B)$ defines a conditional probability). Which is the probability to get an even number in a dice roll?

For the answer this question, we must to consider: $A \xrightarrow{\text{event}}$ dice roll and $B \xrightarrow{\text{event}}$ get a even number. Hence,

$$P(A|B) = \frac{3}{6} = \frac{1}{2} = 50\%. \tag{1.15}$$

[3]See, CM is a deterministic theory. If we have a initial condition of all universe's particles plus Newton's laws we could compute all future and development of nature.

Exercise 1.13: Exponential of Operators

Prove that, for any linear operator A

$$A^n A^m = A^{n+m},$$

holding for $\{n, m\} \in \mathbb{R}$.

Exercise 1.14: Bell-Wigner Inequality

Prove the Bell-Wigner Inequality.

Exercise 1.15: Moments of Binomial Distribution

Show that,

$$\langle n \rangle = Np, \quad \left\langle (\Delta n)^2 \right\rangle = Np(1-p).$$

for a binomial distribution.

Exercise 1.16: Moments of Gaussian Distribution

Show that, for a distribution

$$p(x) := (\sigma^2 2\pi)^{-1/2} \exp\left(-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right),$$

we have

$$\langle X \rangle = \mu, \quad \left\langle (\Delta X)^2 \right\rangle = \sigma^2.$$

Exercise 1.17: Law of Large Numbers

1. Assuming the probability of obtaining “heads” in a coin toss in 0.5, compare the probability of obtaining “heads” in 5 out of 10 tosses with the probability of obtaining “heads” in 50 out of 100 tosses.

2. For a set of 10 tosses and for a set of 100 tosses, calculate the probability that the fraction of “heads” will be between 0.445 and 0.555.

1.5 Select problems

Exercise 1.18: Functon Space

Consider the vector space that consists of all possible linear combinations of the following functions: 1, $\sin(x)$, $\cos(x)$, $\sin^2(x)$, $\cos^2(x)$, $\sin(2x)$, and $\cos(2x)$. What is the dimension of this space? Exhibit a possible set of basis vectors, and demonstrate that it is complete.

Exercise 1.19: Pauli Matrices

Since a linear combination of two matrices of the same shape is another matrix of that shape, it is possible to regard matrices as members of a linear vector space. Show that any 2×2 matrix can be expressed as a linear combination of the following four matrices $\mathbb{1}_2$, $\{\sigma_i\}_{i=x,y,z}$.

Exercise 1.20: Inner Product of Matrices

If A and B are matrices of the same shape, show that $(A, B) = \mathrm{Tr}\left(A^\dagger B\right)$ has all of the properties of an inner product. Hence show that the four matrices of the problem 1.5 are orthogonal with respect to this inner product.

Exercise 1.21: Symmetrizer and Antisymmetrizer Operators

Show that the symmetrizer S, defined for an arbitrary function $\phi(x)$ as $S\left(f(x)\right) = \frac{1}{2}\left[\phi(x) + \phi(-x)\right]$, and the antisymmetrizer A, defined as $A\left(\phi(x)\right) = \frac{1}{2}\left[\phi(x) - \phi(-x)\right]$, are projection operators.

Exercise 1.22: Functions of Operators

Using he definition of a function operator, $f(A) = \sum_i f(a_i) \left|a_i\right\rangle\!\left\langle a_i\right|$, with $A\left|a_i\right\rangle = a_i\left|a_i\right\rangle$ and $\left\langle a_i|a_j\right\rangle = \delta_{ij}$, prove that the power function $f_n(A) \equiv A^n$ satisfies the relation $\left(A^n\right)\left(A^m\right) = A^{n+m}$.

Exercise 1.23: Hilbert and Function Spaces

1. Consider a Hilbert space $\mathcal{H}$ that consists of all functions $\psi = \psi(x)$ such that
$$\int_{-\infty}^{+\infty} \mathrm{d}x\, |\psi|^2 < \infty.$$
Show that there are functions space Ω which $Q\psi \equiv x\psi$ is not in $\mathcal{H}$.

2. Consider the function space Ω which consists of all $\phi = \phi(x)$ that satisfy the infinite set of conditions,
$$\int_{-\infty}^{+\infty} \mathrm{d}x\, |\phi|^2 (1 + |x|^2) < \infty. \quad \text{for } n = 0, 1, 2, \cdots.$$
Show that any $\phi(x)$ in Ω the function $Q\phi \equiv x\phi$ is also in Ω.

Exercise 1.24: Extended Space $\Omega^{\times}$

The extended space $\Omega^{\times}$ consists of those functions $\chi(x)$ which satisfy the condition

$$(\chi, \phi) = \int_{-\infty}^{+\infty} \mathrm{d}x\, \chi^{*}(x)\phi(x) < \infty \qquad \forall \phi \in \Omega.$$

The nuclear space Ω and the Hilbert space $\mathcal{H}$ have been defined in the previous problem. Which of the following functions belong to Ω, to $\mathcal{H}$, and/or to $\Omega^{\times}$? (a)$\sin(x)$; (b)$\sin(x)/x$; (c)$x^2\cos(x)$; (d)$\exp(-ax)(a > 0)$; (e)$[\log(1+|x|)]/(1+|x|)$; (f)$\exp\left(-x^2\right)$; (g)$x^4\exp(-|x|)$.

Exercise 1.25: Hermiticity of Laplacian

What boundary conditions must be imposed on the functions $\{\phi(\mathbf{x})\}$, defined in some finite or infinite volume of space, in order that the the Laplacian operator be Hermitian?

Exercise 1.26: Equality of Operators

Let $\langle\psi|A|\psi\rangle = \langle\psi|B|\psi\rangle$ for all ψ. Prove that $A = B$, in the sense that $\langle\phi_1|A|\phi_2\rangle = \langle\phi_1|B|\psi_2\rangle$ for all ϕ_i $(i = 1, 2)$.

Exercise 1.27: Star and Planets

The number of stars in our galaxy is about $N = 10^{11}$. Assume that: the probability that a star has planets is $p = 10^{-2}$, the probability that the conditions on a planet are suitable condition, is $r = 10^{-2}$

1. What is the probability of life existing in an arbitrary solar system?

2. What is the probability that life exist in at least one solar system?

Exercise 1.28: Lifetimes and Decay

The probability density for decay of a radioactive nucleus is $P(t) = \alpha e^{-\alpha t}$, where $t \geqslant 0$ is the (unpredictable) lifetime of the nucleus, and α^{-1} is the mean lifetime for such a decay process. Calculate the probability density for $|t_1 - t_2|$, where t_1 and t_2 are the lifetimes of two such identical independent nuclei.

Exercise 1.29: Independent Variables

Let $\{X_n\}$ be a mutually independent random variables, each of which has the probability density

$$\begin{aligned} P_1(x) =& \alpha e^{-\alpha x} \quad (x \geqslant 0) \\ =& 0 \quad (x < 0) \end{aligned}$$

under some condition C. That is to say, $P(x < X_j < x + \mathrm{d}x \,|C) = P_1(x)\,\mathrm{d}x$ for $1 \leqslant j \leqslant n$. Show that the probability density for the sum of these variables, $S = \sum\limits_n X_n$, is

$$P_n(x) = \alpha(\alpha x)^{n-1} e^{-\alpha x}/(n-1)!.$$

Exercise 1.30: Particle Source

A source emits particles at an average rate of λ particles per second; however, each emission is stochastically independent of all precious emission events. Calculate the probability that exactly n particles will be emitted within a time interval t

1.6 Solutions

In this section, we will dedicate ourselves to solving some the exercises of studied chapter.

1.6.1 Exercise 1.1:

Yes. The complex number, define as $z = x + iy$, where $\{x, y\} \in \mathbb{R}$, are elements of a vector space (V) of dimension two.

Proof. To prove the last preposition we have to verify that:

1. let be $z_i = x_i + iy_i$ with $\{J_i\}_{i=1,2}^{J=x,y}$ any reals scalars. Then, $(z_1 + z_2) \in V$, i.e. V is closed to sum;
2. for any $z \in V$ and μ (a scalar), we have an element $(\mu z) \in V$;
3. exist a null element (e.g., $z + \bar{0} = z \, \forall(z) \in V$) such that $\bar{0} \in V$.

Firstly, we have:

$$\begin{aligned} z_1 + z_2 =& x_1 + iy_1 + x_2 + iy_2 \\ =& \underbrace{(x_1 + x_2)}_{\text{scalar}}(1) + \underbrace{(y_1 + y_2)}_{\text{scalar}}(i), \end{aligned}$$

therefore, the requirement hold for any $(z_i + z_j)$. On about the second prerequisite:

$$\mu z_i = \mu x_1(1) + \mu y_i(i) \equiv z_k$$

holding for any μ $(z_k \in V)$. Finally, for the last condition

$$\bar{0} \equiv 0(1) + (0)i,$$

then $\bar{0} \in V$. $\square$

1.6.2 Exercise 1.2

Proof. Hypothesis: $c_1(\sin(2x)) + c_2(\sin(x)) = 0$ hold if, and only if, $c_1 = c_2 = 0$. Then, $\{\sin(2x), \sin(x)\}$ are linearly independent.

By a directly evaluation of above hypothesis, we have:

$$
\begin{aligned}
c_1(2\cos(x)\sin(x)) &= -\, c_2 \sin(x) \\
c_1 \cos(x) = -c_2 \quad &\text{or} \quad c_1 = c_2 = 0,
\end{aligned}
$$

nevertheless, the above condition must be satisfied for any $x \in \mathcal{D}(V)$ (x in domain of the functionals). Therefore, due to the $\cos(x)$ is not constant for all $x \in \mathcal{D}(V)$, then a unique solution it is $c_1 = c_2 = 0$. □

1.6.3 Exercise 1.3

Proof. Let

$$
(\psi(x), \phi(x)) := \int_{\mathcal{D}(V)} \mathrm{d}x\, \psi^*(x)\phi(x),
$$

be the definition of the inner product in the space of differential functions.

Evaluating $(\sin(2x), \sin(x))$ we get

$$
(\sin(2x), \sin(x)) = 2\int_{\mathcal{D}(V)} \mathrm{d}x \cos(x)\sin^2(x).
$$

Now, via the following change of variable $u = \sin(x)$ ($\mathrm{d}x\cos(x) = \mathrm{d}u$, $\mathcal{D}(V) \to \mathcal{D}_u$) we have

$$
\begin{aligned}
(\sin(2x), \sin(x)) =& 2\int_{\mathcal{D}_u} \mathrm{d}u\, u^2 \\
=& 2/3\left[u^3 + C\right]_{\mathcal{D}_u} \\
=& 2/3\left[\sin^3(x) + C\right]_{\mathcal{D}(V)}.
\end{aligned}
$$

In general, due to the periodicity of the trigonometric functions in question, we can set $\mathcal{D}(V) = [0, 2\pi)$. Hence, $(\sin(2x), \sin(x)) = 0$ for all $x \in [0, 2\pi)$. Thus, we conclude that $\{\sin(2x), \sin(x)\}$ are an orthogonal set (as we can see by Theorem 1.1). □

1.6.4 Exercise 1.4

Proof. For this proof, we shall start with a consideration: every vector in a linear vector space (e.g., $\psi \in (V)$) can be decomposed into two components,

$$\psi := \chi + P_\psi(\phi), \tag{1.16}$$

where $P_\psi(\phi)$ is the projection of any $\phi \in V$ into the ψ-subspace of V (i.e., $P_\psi(\phi) \in V^\psi$) and χ an element of orthogonal subspace of V^ψ (which can be represented as $V_\perp^\psi$). Because of last definition, (1.16), we can use Gram–Schmidt process to written:

$$\chi = \psi - \frac{(\psi, \phi)}{(\phi, \phi)}\phi, \tag{1.17}$$

an orthogonal vector to ϕ ($\phi \neq 0$). Moreover, due orthogonal condition between ϕ and χ, we have

$$\begin{aligned} \|\psi\|^2 =& \frac{|(\psi, \phi)|^2}{\|\phi\|^2} + \underbrace{\|\chi\|^2}_{\geqslant 0} \\ \geqslant& \frac{|(\psi, \phi)|^2}{\|\phi\|^2}. \end{aligned} \tag{1.18}$$

Now, for $\phi = 0$, we can compute directly: $(\psi, \phi = 0) = \|\psi\|(0)$.

Hence, the Cauchy-Schawarz's inequality (CSI)

$$|(\psi, \phi)|^2 \leqslant \|\psi\|^2 \|\phi\|^2,$$

hold for any pair $\{\psi, \phi\} \in V$. □

1.6.5 Exercise 1.5

Proof. The norm square of $\psi + \phi$ ($\{\psi, \phi\} \in V$) could be computed via

$$\begin{aligned} \|\psi + \phi\|^2 =& (\psi, \psi) + (\phi, \phi) + (\phi, \psi) + (\psi, \phi) \\ =& \|\psi\|^2 + \|\phi\|^2 + 2\,\mathrm{Re}\{(\psi, \phi)\}, \end{aligned}$$

And, by virtue of CSI[4], we rewrite the above equation as follows:

$$\|\psi + \phi\|^2 \leqslant \|\psi\|^2 + \|\phi\|^2 + 2\|\psi\|\|\phi\|,$$

[4] Refer to the preceding exercise.

therefore, we conclude

$$\|\psi + \phi\| \leqslant \|\psi\| + \|\phi\|. \tag{1.19}$$

□

1.6.6 Exercise 1.6

Let $A \doteq \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ be a a matrix representation of a linear operator A. Then, $A\psi = \phi$.

Proof. Evaluating $A\psi$, we obtain

$$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} 3 \\ 2 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}.$$

Moreover, we can prove that A is a linear operator:

1. let $u \doteq (a_1, b_1, c_1)^\intercal$ and $v \doteq (a_2, b_2, c_2)^\intercal$ be generic vectors in domains of A, and $\{\lambda_{1,2}, a_{1,2}, b_{1,2}, c_{1,2}\}$ scalars, we have

   $$A(\lambda_1 u + \lambda_2 v) \doteq \lambda_1 \begin{pmatrix} c_1 \\ 0 \\ c_1 \end{pmatrix} + \lambda_2 \begin{pmatrix} c_2 \\ 0 \\ c_2 \end{pmatrix},$$

   $$A(u) \doteq \begin{pmatrix} c_1 \\ 0 \\ c_1 \end{pmatrix} \quad A(v) \doteq \begin{pmatrix} c_2 \\ 0 \\ c_2 \end{pmatrix},$$

   therefore, concatenating the equations above, we show that

   $$A(\lambda_1 u + \lambda_2 v) = \lambda_1 A(u) + \lambda_2 A(v).$$

   Hence, A is a linear operator.

□

1.6.7 Exercise 1.7

Proof. Computing $\partial_x(x\psi)$, where $\psi = \exp(x)$, we obtain

$$\left(\frac{\partial}{\partial x}x\right) = (\exp(x))\,(1+x)\exp(x),$$

hence, $\partial_x(x\psi) = (1-x)\psi$. Then, ψ is an eigenfunction of $\partial_x x$ with eigenvalue $a(x) = 1 + x$. $\square$

1.6.8 Exercise 1.8

Proof. Due to the Hermitian conjugation (HC) symmetry and associative proprieties, we have for any $\{|\psi\rangle, |\phi\rangle, |\alpha\rangle, |\beta\rangle\} \in \mathcal{H}$

$$\begin{aligned}
\langle\psi|(|\alpha\rangle\langle\beta|)|\phi\rangle &= \langle\alpha|\psi\rangle^* \langle\phi|\beta\rangle^* \\
&= (\langle\phi|\beta\rangle\langle\alpha|\psi\rangle)^* \\
&= (\langle\phi|(|\beta\rangle\langle\alpha|)|\psi\rangle)^* \\
&\equiv \underbrace{\Big(\langle\phi|(|\alpha\rangle\langle\beta|)^\dagger|\psi\rangle\Big)^*}_{\text{By definition}}
\end{aligned}$$

therefore,

$$(|\alpha\rangle\langle\beta|)^\dagger = |\beta\rangle\langle\alpha| \qquad \forall\{|\alpha\rangle, |\beta\rangle\},$$

as shown in (1.10). $\square$

1.6.9 Exercise 1.9

Proof. Let $\mathcal{B}_k = \{|\phi_i^k\rangle\}$ $(i = 1, \cdots, \dim(\mathcal{H}))$ denoted an orthonormal k-basis for a Hilbert space $\mathcal{H}$[5]. For two different basis indexed by $\{k, k'\}$ we have

$$\left\langle \phi_i^k \middle| \phi_j^{k'} \right\rangle := \delta_{ij}\delta_{kk'}. \tag{1.20}$$

[5]Note that is a general case. For each set of basis $\{A_K\}$, we determine, for instance, through the Gram-Schmidt orthogonalization procedure, a set of orthonormal basis as well as addressing the given problem.

Evaluating $\operatorname{Tr} O$, where $O \in \mathcal{H}$, we obtain:

$$\begin{aligned}
\operatorname{Tr} O &= \operatorname{Tr}[O]_{\mathcal{B}_k} \\
&= \sum_i \left\langle \phi_i^k \middle| O \middle| \phi_i^k \right\rangle \\
&= \sum_i \langle \phi_i^k | \left[\left(\sum_j \left| \phi_j^{k'} \middle\rangle\!\middle\langle \phi_j^{k'} \right| \right) O \left(\sum_v |\phi_v^u\rangle\langle\phi_v^u| \right) \right] |\phi_i^k\rangle \\
&= \sum_i \langle \phi_i^k | \left(\sum_{j,v} \left\langle \phi_j^{k'} \middle| O \middle| \phi_v^u \right\rangle \left| \phi_j^{k'} \middle\rangle\!\middle\langle \phi_v^u \right| \right) |\phi_i^k\rangle \\
&= \sum_{i,j,v} \left\langle \phi_j^{k'} \middle| O \middle| \phi_v^u \right\rangle \underbrace{\left\langle \phi_i^k \middle| \phi_j^{k'} \right\rangle}_{\delta_{ij}\delta_{kk'}} \underbrace{\left\langle \phi_v^u | \phi_i^k \right\rangle}_{\delta_{vi}\delta_{uk}} \\
&= \sum_j \left\langle \phi_j^{k'} \middle| O \middle| \phi_j^{k'} \right\rangle \\
&= \operatorname{Tr}[O]_{\mathcal{B}_j} .
\end{aligned}$$

□

1.6.10 Exercise 1.10

From the characteristic equation, we have

$$\det A = \lambda_n(2 - \lambda_n^2) = 0 \implies \lambda_n = \left(1, \sqrt{2}, -\sqrt{2}\right),$$

where $\{\lambda_n\}$ are the eigenvalues of A.

Now, we shall determine the eigenvectors corresponding to each λ_n. For the first ($\lambda_1 = 0$), we obtain

$$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} a_1 \\ b_1 \\ c_1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \therefore |u_1\rangle \doteq a_1 \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix},$$

where $|u_1\rangle \doteq 1/\sqrt{2}(1, 0, -1)^\intercal$ is the normalized eigenvector associates to λ_1.

in same way of previous discussion, for $\lambda_{2,3}$

$$\begin{pmatrix} \mp\sqrt{2} & 1 & 0 \\ 1 & \mp\sqrt{2} & 1 \\ 0 & 1 & \mp\sqrt{2} \end{pmatrix} \begin{pmatrix} a_i \\ b_i \\ c_i \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \therefore |u_2\rangle \doteq \frac{1}{2} \begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix}; |u_3\rangle \doteq \frac{1}{2} \begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix}$$

defining the normalized eigenvectors $\{|u_2\rangle, |u_3\rangle\}$.

1.6.11 Exercise 1.11

For the first Theorem:

Proof. Hypothesis (HP): $\langle\psi|A|\psi\rangle = (\langle\psi|A|\psi\rangle)^*$ for all $|\psi\rangle$, Then $A = A^\dagger$.

Let $\mathcal{B} = \{|i\rangle\}$ be a basis of $\mathcal{H}$. Then any *ket* can be decomposed into $|\psi\rangle = \sum_i c_i |i\rangle$, in this context we obtain

$$\langle\psi|A|\psi\rangle = \sum_i |c_i|^2 \underbrace{\langle i|A|i\rangle}_{\equiv A_{ii}}.$$

Furthermore, via complex conjugation of the above equation

$$\begin{aligned}(\langle\psi|A|\psi\rangle)^* &= \sum_i |c_i|^2 A_{ii}^* \\ &\equiv \underbrace{\sum_i |c_i|^2 A_{ii},}_{\text{HP}}\end{aligned}$$

therefore, $A_{ii} = A_{ii}^*$ which implies $[A]_{\mathcal{B}} = [A^\dagger]_{\mathcal{B}}$. □

For the second Theorem:

Proof. By assuming that A is Hermitian ($A = A^\dagger$), we can derive the equation $\langle\phi| A = a^* \langle\phi|$ when applying the Hermitian conjugation to the eigenvalue equation $A|\phi\rangle = a|\phi\rangle$.

Hence,

$$\begin{cases}\langle\phi|A|\phi\rangle = \ \ a\langle\phi|\phi\rangle \\ \langle\phi|A|\phi\rangle = a^*\langle\phi|\phi\rangle\end{cases}$$

or, subtracting the above equations, we obtain

$$(a - a^*)\langle\phi|\phi\rangle = 0, \tag{1.21}$$

therefore, the solution for all $|\phi\rangle$ is $a = a$ that implies $a \in \mathbb{R}$ □

For the last Theorem:

Proof. For any eigenvectors $\{|\phi_i\rangle\}$ of a Hermitian operator A we have $A|\phi_i\rangle = a_i|\phi_i\rangle$ and $|\phi_j\rangle A = a_j|\phi_j\rangle$, where $a_k \in \mathbb{R}$ (Theorem 1.6). Then,

$$\begin{cases} \langle\phi_j|A|\phi_i\rangle = a_i\langle\phi_j|\phi_i\rangle \\ \langle\phi_i|A|\phi_i\rangle = a_j\langle\phi_i|\phi_j\rangle \end{cases}$$

and due to the Hermitian conjugation symmetry, we rewritten the above equations as follows

$$(a_j - a_i)\langle\phi_i|\phi_j\rangle = 0.$$

However, $a_i \neq a_j$ (hypothesis of Theorem 1.7) which implies that $\langle\phi_i|\phi_j\rangle = 0$ (i.e., the eigenkets of A corresponding to different eigenvalues are orthogonal). $\square$

1.6.12 Exercise 1.12

Let $P_i = \sum_{j=1}^{d} |\phi_{ij}\rangle\langle\phi_{ij}|$ be a projector operator. We shall see that

1. P is Hermitian;

   Proof.

   $$\begin{aligned} P^\dagger &= \left(\sum_{j=1}^{d} |\phi_{ij}\rangle\langle\phi_{ij}|\right)^\dagger \\ &= \sum_{j=1}^{d} \left(|\phi_{ij}\rangle\langle\phi_{ij}|\right)^\dagger \\ &= P, \end{aligned}$$

   where we used (1.10) (see Exercise 1.8) $\square$

2. P is idempotent;

Proof.

$$
\begin{aligned}
P^2 &= \sum_{j=1}^{d} |\phi_{ij}\rangle\langle\phi_{ij}|^{\dagger} \left(\sum_{k=1}^{d} |\phi_{lk}\rangle\langle\phi_{lk}| \right) \\
&= \sum_{j,k} \langle\phi_{ij}| \underbrace{(\langle\phi_{ij}|\phi_{lk}\rangle)}_{\delta_{li}\delta_{kl}} |\phi_{lk}\rangle \\
&= \sum_{j=1}^{d} |\phi_{ij}\rangle\langle\phi_{ij}| \\
&= P
\end{aligned}
$$

□

1.6.13 Exercise 1.13

See the solution of Exercise 1.22.

1.6.14 Exercise 1.14

Proof. To initiate this proof, let us first consider the number of possibilities available. If the probability on the left-hand side is non-null, it follows that $A_1 = C_2 = +$, which in turn implies $B_1 = +$ (or $B_2 = +$). In this context, both sides of the Bell-Wigner equation are equal in terms of probability.

On the other hand, if we assume $A_1 = B_2 = +$, then $P(A_1\&B_2) > 0$. However, we can find a situation where $C_2 = -$, implying that $P(A_1\&B_2) > P(A_1\&C_2)$. In general, the inequality can be expressed as:

$$P(A_1\&C_2) \leqslant P(B_1\&C_2) + P(A_1\&B_2).$$

□

1.6.15 Exercise 1.15

For the mean value prove:

Proof. the mean value $\langle n \rangle$ can be computed via

$$\langle n \rangle = \sum_{r=0}^{N} r \frac{N!}{r!(N-r)!} p^r q^{N-r},$$

where r is the ratio of obtain n in a measure of an event E, N is total number of measures, p the probability to get n and q is defined as non-p (i.e. $p + q = 1$). Moreover, it is important to note that

$$p\partial_p p^r = rp^r.$$

Now, rewritten the first equation, we obtain

$$\begin{aligned}\langle n \rangle =& p\partial_p \underbrace{\sum_{r=0}^{N} \frac{N!}{r!(N-r)!} p^r q^{N-r}}_{=(p+q)^N} \\ =& p\frac{\partial}{\partial p}^N \\ =& Np(p+q)^{N-1} \\ =& Np.\end{aligned}$$

where in the first line we used the sum over all probabilities must to be one.

□

For the second moment:

Proof. Before we looking at the second moment, let us make some consideration on $\langle n^2 \rangle$:

$$\begin{aligned}\langle n^2 \rangle =& p\partial_p \left[p\partial_p \left(\sum_{r=0}^{N} \frac{N!}{r!(N-r)!} p^r q^{N-r} \right) \right] \\ =& p\partial_p \left(Np(p+q)^{N-1} \right) \\ =& N^2p^2 + Np - Np^2.\end{aligned}$$

Therefore, when we evaluate $\langle (\Delta n)^2 \rangle$, we obtain

$$\begin{aligned}\langle (\Delta n)^2 \rangle =& N^2p^2 + Np - Np^2 - N^2p^2 \\ =& Np(1-p).\end{aligned}$$

□

1.6.16 Exercise 1.16

At the first, we want to show that $\langle X \rangle = \mu$.

Proof. Evaluating the expectation value of x in terms of a new variable $k = x - \mu$ ($\mathrm{d}k = \mathrm{d}x$), we obtain

$$\begin{aligned}\langle X \rangle =&(\sigma^2 2\pi)^{-1/2} \int_{-\infty}^{+\infty} \mathrm{d}k\,(k+\mu) \exp\left(-\frac{k^2}{2\sigma^2}\right) \\ =&(\sigma^2 2\pi)^{-1/2} \left[\mu \underbrace{\int_{-\infty}^{+\infty} \mathrm{d}k \exp\left(-\frac{k^2}{2\sigma^2}\right)}_{\sqrt{\sigma^2 2\pi}} + \underbrace{\int_{-\infty}^{+\infty} \mathrm{d}k\, k \exp\left(-\frac{k^2}{2\sigma^2}\right)}_{=0,\text{ odd int.}} \right] \\ =&\mu.\end{aligned}$$

$\square$

On demonstration of $\left\langle (\Delta X)^2 \right\rangle = \sigma^2$:

Proof. By the definition of variance, we have

$$\begin{aligned}\left\langle (\Delta X)^2 \right\rangle =&\left\langle (x - \langle X \rangle)^2 \right\rangle \\ =&\left\langle x^2 \right\rangle - \langle x \rangle^2 \\ =&-\mu^2 \left(\frac{\alpha}{\pi}\right)^{1/2} \int_{-\infty}^{+\infty} \mathrm{d}k\,(k+\mu)^2 \exp\left(-\alpha k^2\right) \\ =&\left(\frac{\alpha}{\pi}\right)^{1/2} \left(-\frac{\mathrm{d}}{\mathrm{d}\alpha}\right) \int_{-\infty}^{+\infty} \mathrm{d}k\, k^2 \exp\left(-\alpha k^2\right) \\ =&\left(\frac{\alpha}{\pi}\right)^{1/2} \frac{\sqrt{\pi}}{2} \left(\frac{1}{\alpha}\right)^{3/2} \\ =&\sigma^2,\end{aligned}$$

where we used $\alpha \equiv (2\sigma^2)^{-1}$. $\square$

1.6.17 Exercise 1.17

On the probability to obtain heads five times in ten tosses:

$$P(\text{head} = 5|(\text{Toss})^{10}) = \frac{10!}{5!5!}(0.5)^5(0.5)^5 = 0.246 \approx 25\%.$$

On fifty heads in one hundred tosses:

$$P(\text{head} = 50|(\text{Toss})^{100}) = \frac{100!}{50!50!}(0.5)^{50}(0.5)^{50} = 0.0796 \approx 8\%.$$

Hence, due to the above equations, we could see the *Law of Large Numbers*. Means that, for a large number of execution (same experiment) a probability of a specific event happens decay.

1.6.18 Exercise 1.18

In this exercise we prove that a set $\{1, \cos(x), \sin(x), \cos(2x), \sin(2x)\}$ are orthogonal. Then, the Hilbert space in question has $\dim \mathcal{H} = 5$

Proof. Step 1: Due to the fundamental law of trigonometry

$$\cos^2(x) + \sin^2(x) = 1,$$

therefore, the set $\mathcal{B}_1 = \{\{1\}, \{\cos^2(x), \sin^2(x)\}\}$ are not an orthogonal set.

Step 2: The square cosine function of double arch can be written as follows:

$$\begin{aligned}\cos(2x) &= \cos^2(x) - \sin^2(x) \\ &= \cos^2(2x) - 1 + \cos^2(x) \\ &= 2(\cos^2(x)) - 1(1),\end{aligned}$$

hence, $\mathcal{B}_2 = \{\{1\}, \{\cos(2x), \cos^2(x)\}\}$ are not a L.I. set.

Step 3: From the Exercise 1.2 we prove that $\{\sin(2x), \sin(x)\}$ are a L.I. set. Then, a possible orthogonal set are $\mathcal{B}_3 = \{\{1\}, \{\sin(x), \sin(2x)\}\}$. Evaluating the inner product (IP) between 1 and $\sin(x)$, we obtain

$$(1, \sin(x)) = \int_0^{2\pi} \mathrm{d}x \sin(x) = 0 \tag{1.22}$$

then $\mathcal{B}_3$ are an orthogonal set.

Step 4: If we compute $(\sin(x), \cos(x))$, we have

$$(1, \cos(mx)) = \int_0^{2\pi} \cos(mx) = \left[\frac{\sin(mx)}{m}\right]_0^{2\pi} = 0, \tag{1.23}$$

hence, $\mathcal{B}_4 = \{1, \cos(x), \cos(2x), \sin(x), \sin(x)\}$ are an orthogonal. □

1.6.19 Exercise 1.19

Any matrix $M \in \mathcal{M}_2(\mathbb{C})$ can be written as linear combination of $\{E_{ij}\}_{ij=1,2}$, where E_{ij} is a (2×2)-matrix with a 1 in the ith row, jth column and zeros everywhere else.

Proof. Let $\mathcal{S} = \{\{c_k\}_{k=1,\cdots,4} | c_i \in \mathbb{C}\}$ denotes the elements of $M \in \mathcal{M}_2(\mathcal{C})$. Then,

$$\begin{aligned} M(\mathbb{C}) =& c_1 E_{11} + c_2 E_{12} + c_3 E_{21} + c_4 E_{22} \\ =& \begin{pmatrix} c_1 & c_2 \\ c_3 & c_4 \end{pmatrix}. \end{aligned}$$

Hence, $\dim(\mathcal{M}_2) = 4$. □

Due to the $\dim(\mathcal{M}_2) = 4$ and $\mathcal{B} = \{\mathbb{1}, \{\sigma_i\}_{i=x,y,z}\}$ a set of four linearly independent elements, thus $\mathcal{B}$ is a basis for $\mathcal{M}_2$. In other words, each element $M \in \mathcal{M}_2$ can be written in $\mathcal{B}$ basis.

Proof. To prove the linearly independence of $\mathcal{B}$, we have to consider:

$$a_0 \infty_2 + \sum_{i=1}^{3} a_i \sigma_i = 0$$

or, in other words

$$\begin{cases} a_0 + a_3 = 0 \\ a_1 - i c_2 = 0 \\ c_1 + i c_2 = 0 \\ c_1 - c_3 = 0 \end{cases}$$

which implies that $a_j = 0$ for all $j = 0, \cdots, 3$. Therefore, $\mathcal{B}$ is a basis and every vector in 2-square matrix space can be express as linear combination of $\mathcal{B}$ elements.

□

1.6.20 Exercise 1.20

To prove that $\mathrm{Tr}\left(A^\dagger B\right)$ can express formally an internal product we have to verify:

1. could it $(A, \lambda_1 B + \lambda_2 C) = \lambda_1 (A, B) + \lambda_2 (A, B)$ hold for any operators A, B, C and scalars $\{\lambda_j\}$ $(j = 1, 2)$?

Proof.

$$\begin{aligned}(A, \lambda_1 B + \lambda_2 C) =& \operatorname{Tr}\left[A^\dagger\left(\lambda_1 B + \lambda_2\right)\right] \\ =& \lambda_1 (A, B) + \lambda_2 (A, B),\end{aligned}$$

which holds in any case, specially, because of the distributive and associativity proprieties of matrix. □

2. the IP between sames elements defines a norm measure as follows $(A, A) \geqslant 0$.

   Proof. Evaluating the above discussion, we obtain

$$\begin{aligned}(A, A) =& \operatorname{Tr}(A^\dagger A) \\ =& \sum_i (A_{ii}^*) (A_{ii}) \\ =& \sum_i |A_{ii}|^2 \\ \geqslant& 0, \quad \forall A\end{aligned}$$

   where A_{ii} denotes the ith diagonal-element of A. □

   which prove that $(A, B) = \operatorname{Tr}(A^\dagger B)$ can used as a form of internal product in matrix space.

1.6.21 Exercise 1.21

First, looking at the symmetrizer operator, we have: $S^2\left(f(x)\right) \equiv S\left[S\left(f(x)\right)\right] = S\left(f(x)\right)$ (*idempotent*)

Proof.

$$\begin{aligned}S^2(\phi) =& \frac{1}{2}\left[S(\phi)(x) + S(\phi)(-x)\right] \\ =& \frac{1}{2}\left[\frac{1}{2}\left((\phi(x) + \phi(-x)\right) + \frac{1}{2}\left(\phi(-x) + \phi(x)\right)\right] \\ =& \frac{1}{2}\left(\phi(x) + \phi(-x)\right) \\ =& S(\phi) \quad \forall \phi(x).\end{aligned}$$

□

Then, $S(\cdot)$ is a projector operator since subsequent applications of S give us the same result, which is very similar to the projectors operators P defined in the last chapter (less than Hermiticity, which hold under $\mathcal{D}(\phi) = \mathbb{R}$).

Now, focus in antisymmetrizer operator, we obtain a very similar result:

$$\begin{aligned} A^2(\phi) =& \frac{1}{2}\left[A(\phi)(x) - A(\phi)(-x)\right] \\ =& \frac{1}{2}\left[\frac{1}{2}\left((\phi(x) - \phi(-x)\right) - \frac{1}{2}\left(\phi(-x) - \phi(x)\right)\right] \\ =& A(\phi) \quad \forall \phi(x). \end{aligned}$$

1.6.22 Exercise 1.22

Proof. Computing $(A)^n(A)^m |\psi\rangle$ and using $f(A) = \sum_i f(a_i) |a_i\rangle\langle a_i|$, we obtain:

$$\begin{aligned} (A)^n(A)^m |\psi\rangle =& (A)^n(A)^m \left(\sum_j |a_j\rangle\langle a_j|\right) |\psi\rangle \\ =& \sum_j (A)^n \left((a_j)^m |a_j\rangle\langle a_j|\right) |\psi\rangle \\ =& \left(\sum_j (a_j)^n (a_j)^m |a_j\rangle\langle a_j|\right) |\psi\rangle \\ =& \left(\sum_j (a_j)^{n+m} |a_j\rangle\langle a_j|\right) |\psi\rangle \\ \equiv& A^{n+m} |\psi\rangle, \quad \forall |\psi\rangle \end{aligned}$$

which implies that $A^n A^m = A^{n+m}$, for all $|\psi\rangle$. □

1.6.23 Exercise 1.23

1. The eigenfunction of position in p-space (momentum space) can be written as follows

$$(-i\hbar\partial_p)\,\overline{\psi}(p).$$

Then, a eigenfunctions are formally defined as

$$\overline{\psi}(p) = \exp(-ipx/\hbar),$$

moreover, due to the Fourier Transform

$$\begin{aligned}\psi(x) =& \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty} \mathrm{d}p \exp\bigl(-ip(x-x')\bigr)\\ =&\delta(x-x').\end{aligned}$$

Therefore, $\psi(x)$ is not a limited function (i.e. $\psi(x) \notin \mathcal{H}$).

Proof.

$$(\psi(x), \psi(x)) = \int_{-\infty}^{+\infty} \mathrm{d}x\, \delta(x-x')^2 \approx +\infty,$$

which means that $\psi(x)$ has non-limited norm. Thus, $\psi(x) \notin \mathcal{H}$. □

2. Evaluating the condition $Q\phi \in \Omega$ we shall see that hold for any $\phi(x)$.

Proof.

$$\begin{aligned}\int_{-\infty}^{+\infty} \mathrm{d}x\, |x\phi|^2 \left(1+|x|^n\right) =& \int_{-\infty}^{+\infty} \mathrm{d}x\, |\phi|^2 \left(2-2+|x|^2+|x|^{n+2}\right)\\ =& \int_{-\infty}^{+\infty} \mathrm{d}x\, |\phi|^2 \left[\left(1+|x|^2\right)+\left(1+|x|^{n+2}\right)\right]\\ &-2\int_{-\infty}^{+\infty} \mathrm{d}x\, |\phi|^2.\end{aligned}$$

However, by our hypothesis, $\phi \in \Omega \subset \mathcal{H}$. Thus,

$$\begin{aligned}&\int_{-\infty}^{+\infty} \mathrm{d}x\, |\phi|^2 \left(1+|x|^2\right) < +\infty;\\ &\int_{-\infty}^{+\infty} \mathrm{d}x\, |\phi|^2 \left(1+|x|^{n+2}\right) < +\infty;\\ &\int_{-\infty}^{+\infty} \mathrm{d}x\, |\phi|^2 < +\infty;\end{aligned}$$

which implies that $Q\phi(x) \in \Omega$ for all $\phi(x)$.

□

1.6.24 Exercise 1.24

Proof.

- $\sin(x) \in \Omega^{\times}$: Since $\phi(x) \in \Omega$ and $\phi(\pm\infty) \to 0$, we have that the scalar product (χ, ϕ) exists for all x. Note, $\sin(x)$ is a limited function and ϕ vanish, so is trivial that $(\sin(x), \phi) < \infty$;

- $\sin(x)/x \in \mathcal{H}$: as $\phi'(x) = \phi(x)/x$, where $\phi(x) \in \Omega$ is not in Ω ($\phi'(x) \notin \Omega$), therefore, $\sin(x)/x \notin \Omega$. However, using integration by parts it is easy to show that $\int_{-\infty}^{\infty} \sin(x)/x$ converges for all x;

- $x^2 \cos(x) \in \Omega^{\times}$: To see this we only need to argue that $\psi' \in \Omega$, where $\phi \in \Omega$. Furthermore, if $\phi' \in \Omega$, due to the limitation of the trigonometric functions, it is evident that $x^2 \cos(x) \in \Omega$;

- The exponential function $\exp(-\alpha x) \notin \mathcal{H}$. To establish we go prove that function is not normalized
$$\int_{-\infty}^{\infty} \mathrm{d}x \, e^{-\alpha x} = \frac{-1}{\alpha} \left(0 - \infty\right);$$

- $g(x) = \log(1 + |x|)/(1 + |x|) \notin \mathcal{H}$: Evaluating an integral with the previous function in integrator we shall see that $g(x)$ is not a normalized function.

- The Gaussian satisfies $\int_{-\infty}^{\infty} \exp\left(-x^2\right) = \sqrt{\pi}$, then $\exp\left(-x^2\right) \in \mathcal{H}$. Moreover, via a simple integration by parts, we conclude that $\exp\left(-x^2\right) \in \Omega$
$$\int_{-\infty}^{\infty} \exp\left(-x^2\right) n^m \qquad \forall m = 0, 1, \cdots;$$

- The $f(x) = \exp(-|x|)$ can be view as an element of Ω. Since $f(\pm\infty) \to 0$ exponentially, the integral of $x^2 \exp(-|x|)$ converges for all x, which implies that $f(x) \in \Omega$.

$\square$

1.6.25 Exercise 1.25

Proof. The Hermitian condition in a volume $V = \int_V \mathrm{d}^3x$ for a $\nabla^2\phi(x)$ can be written as follows

$$\int_V \mathrm{d}^3x \left(\phi^*\nabla^2\phi - \phi\nabla^2\phi*\right) = \int_V \mathrm{d}^3x\, \boldsymbol{\nabla}\cdot\left(\phi^*\boldsymbol{\nabla}\phi - \phi\boldsymbol{\nabla}\phi^*\right) = 0,$$

where we used (without prove) the identity: $\boldsymbol{\nabla}\cdot(\phi^*\boldsymbol{\nabla}\phi) = (\boldsymbol{\nabla}\phi)^*\cdot\boldsymbol{\nabla}\phi + \phi^*\nabla^2\phi$. Moreover, via Gauss's Theorem (statement of flux), the above equation can be rewritten in terms of a surface integral:

$$\iint_S \mathrm{d}\mathbf{S}\left(\phi^*\boldsymbol{\nabla}\phi - \phi\boldsymbol{\nabla}\phi^*\right) = 0.$$

Therefore, for finite volume: $\phi = 0$ in surface or $\boldsymbol{\nabla}\phi$. $\square$

1.6.26 Exercise 1.26

For the solution of this problem, see the solution of Exercise 1.11.

1.6.27 Exercise 1.27

For the first item:

Assuming that the conditions of a star contains a planet (SS), a planet are suitable for life (Q) and the life evolving (R) are independent. Then, the probability of an arbitrary solar system has life is computed as follows

$$P(R\&Q|SS) = pqr = (10^{-2})(10^{-2})(10^{-}-2) = 10^{-6}.$$

In other words, due to the independence among the conditions, the calculation of the required probability is performed through direct multiplication of the probabilities of the events.

For the last question (b), using the above discussion, we can provide the probability of a selected star have no life (P_w)

$$P_W = (1 - pqr)^N,$$

then

$$
\begin{aligned}
\ln P_W =& N\ln(1-pqr) \approx \underbrace{N(-pqr)}_{1^{\text{nd}}\text{order}}\\
P_W \approx& \exp(-pqrN).
\end{aligned}
$$

Therefore, the complementary probability of P_W (i.e. probability of an selected star has life (P)) must be formally defined as follows

$$
\begin{aligned}
P =& 1-P_W\\
\approx& 1-\exp(-pqrN) \approx 1,
\end{aligned}
$$

where we used that $\exp(-pqrN) \ll 1$ ($N = 10^{11}$). Thus, for a large sample space, the probability of each event occurring approaches unity.

1.6.28 Exercise 1.28

The probability density for $Z = |t_1 - t_2|$ is $P_Z(t) = \alpha\exp(-\alpha t)$.

Proof. To prove the above sentence, we will compute the cumulative distribution ($F_Z(t)$) over $Z = |t_1 - t_2|$[6]. In formal way, we have

$$
\begin{aligned}
F_Z(t) =& Pr(Z \leqslant t)\\
=& Pr(|t_1 - t_2| \leqslant t)\\
=& Pr(t_2 \leqslant t_1 \leqslant t + t_2 \cup 0 \leqslant t_1 \leqslant t - t_2)\\
=& \iint\limits_{\mathcal{D}} \mathrm{d}t_2\, \mathrm{d}t_1\, P(t_1,t_2) - \iint\limits_{\mathcal{D}'} \mathrm{d}t_2\, \mathrm{d}t_1\, P(t_1,t_2),
\end{aligned}
$$

where $Pr(\cdot)$ denotes a probability value, $P(t_1,t_2) =$ is a joint probability density, $\mathcal{D}$ and $\mathcal{D}'$ are regions defined as

$$
\begin{cases}
\mathcal{D} = \{(t_1;t_2)|t_2 \leqslant t_1 \leqslant t+t_2; 0 \leqslant t_2 \leqslant +\infty\}\\
\mathcal{D}' = \quad \{(t_1;t_2)|0 \leqslant t_1 \leqslant t-t_2; t \leqslant t_2 \leqslant +\infty\}
\end{cases}
$$

[6]Remember that: the connection among $F_Z(t)$ and the probability density is given $P_Z(t) = \dfrac{\mathrm{d}F_Z(t)}{\mathrm{d}t}$, for all constraints $\{Z,t\}$.

then, returning into $F_Z(t)$, we obtain

$$F_Z(t) = \iint_{\mathcal{D}} \mathrm{d}t_2\, \mathrm{d}t_1\, \alpha^2 \exp(-\alpha(t_1 + t_2)) - \iint_{\mathcal{D}'} \mathrm{d}t_2\, \mathrm{d}t_1\, \alpha^2 \exp(-\alpha(t_1 + t_2)).$$

That integral can be solved analytically (or via symbolic calculus, see Mathematica or Matlab), but, in this note, we only show the final expression:

$$F_Z(t) = 1 - \exp(-\alpha t) \implies P_Z(t) = \alpha \exp(-\alpha t). \quad \forall t > 0$$

□

1.6.29 Exercise 1.29

Proof. We want to prove that $P_n = \alpha(\alpha x)^{n-1} e^{-\alpha x}/(n-1)!$ hold for any $n = 1, \cdots, j$. Firstly, for $n = 1$ we have

$$P_1(x) = \alpha \exp(-\alpha x),$$

which is confirmed by the statement.

Our hypothesis: for $n = k$ is truth. Then, when we compute for $k + 1$ via:

$$\begin{aligned} P_{k+1}(t) &= \int_0^t \mathrm{d}x\, P_k(x) P(t-x) \\ &= \frac{\alpha^{n+1}}{(k-1)!} \exp(-\alpha t) \int_0^t \mathrm{d}x\, x^{k-1} \\ &= \frac{\alpha(\alpha x)^k}{k!} \exp(-\alpha t), \end{aligned}$$

or, swapping $t \to x$ and $(K + 1) \to m$

$$P_m(x) = \frac{\alpha(\alpha x)^{m-1}}{(m-1)!} \exp(-\alpha x).$$

□

1.6.30 Exercise 1.30

To start this problem, let us make some considerations on the probability distribution: Let $P_n(t)$ denotes the probability that we have an emission of n particles in a time interval t.

In this context, if each particle emission during h (a time measure). Then, for m events in $t + h$ times: (1) in t times we have m emission or (2) in h interval had a emission. Formally,

$$P_n(t+h) = P_n(t)(1-\lambda h) + P_{n-1}(t)\lambda h,$$

where λ define the emission rate. Taking $h \to 0$ in the above equation, we obtain a recursive relation between $P_n'(t)$ (derivative of $P_n(t)$) and the probability

$$P_n' = -\lambda P_n + \lambda P_{n-1} \implies P_n(t) = \frac{(\lambda t)^n \exp(-\lambda t)}{n!}.$$

Therefore, the average events in t can be express as follows

$$\begin{aligned}
\langle n \rangle &= \sum_n n P_n(t) \\
&= \exp(-\lambda t) \sum_n n \frac{(\lambda t)^n}{n!} \\
&= \exp(-\lambda t) \lambda t \frac{\mathrm{d}}{\mathrm{d}(\lambda t} \exp(\lambda t) \\
&= \lambda t,
\end{aligned}$$

which confirms the previous assumptions on the emission time.

2 Structure of Quantum Mechanics

2.1 Basic Concepts

Every physical theory involves some basic physical concepts, a mathematical formalism, and set of correspondence etc. A primer objective of a physical theory is describe the *real* word. In this sense, we apply Mathematical methods and tools to obtain a directly correspondence in relation to the nature. However, this aim it is not easy at all, specially in QM.

Deep discussions about the completeness and the neediness of QM are made in the beginning of last century. In 1935 Eistein, Podolsky and Rosen (EPR) are said [4]

> Blá Blá

For EPR, every *good* physical theory has two intrinsically proprieties:

1. Every physical theory has to be *correct*. Thus, all experiment that the theory propose to explain must be explained by the fundamentals concepts of the

theory. Otherwise, if is not possible to explain a experiment results, the theory need to be revised.

2. Every element of *physical reality* has a counter part in the theory. An element of the physical reality is determined via the following criteria:

   > If, without in any way disturbing a system, we can predict with certainty (i.e., with probability equal to unity) the value of a physical quantity, then there exists an element of physical reality corresponding to this physical quantity.

Note that Classical Mechanics satisfy every EPR criterion. In this context, EPR argue that QM cannot be a final word in terms of human physical theory and must be revised (we will see formally that is impossible to obtain, with any precision, the value of the linear momentum and the position at the same time). In their words, the Quantum theory was incomplete and the foundations of this theory must be complete.[1]

A good answer for EPR paradox are given by Bohr. In this paper, Bohr presents the complementary principle, which tell us about the ambiguity of a Classical point of view in quantum realm[2]. Basically, it is impossible to determine with arbitrary precision in the same time the value of two *complementary*[3] quantities, for instance: the position and momentum of an electron. Moreover, Bohr argues that the EPR's definition of physical reality it is not a good assumption once, due to the wave package collapse, it is impossible to get a measure of a Quantum system without disturbing.

The end of the above discussion is due to Bell and his set of inequalities. Bell's works yields a mathematical point of view of a hidden variable limit. After Bell inequalities, specially CHSH inequality, experiments test are made and their results

[1] A priori it is possible to have a kind of *hidden variable* which became QM a complete and correct theory of the natural. So many hidden variables theories was proposed, however, in nowadays, it is proved that it is impossible to complete the QM such that all EPR's criterion was satisfied.

[2] We shall discuss on this topic later.

[3] The formal definition is given latter, see the chapter (CITAR).

are: it is not possible a local e realistic (EPR) hidden variable theory describes all Quantum phenomenons.

Mechanical Aspect

In Classical theory, the *dynamical variables* (elements of physical reality) can have a continuum of values (e.g., The energy of a metal plate under an energetic beam).

Otherwise, we have a gamma of experimental evidences (e.g., the photoelectic effect, Frank-Hertz's experiment, atomic stabilization etc.) that this classical point of view are not the most fundamental principle, therefore, we need a new physical structure (Quantum Mechanics). However, how we can represent the physical reality in QM formalism?

Note: in the last chapter (see Chapter 1) we spend a plenty of time to define the QM environment, in special, to built a formal connection between the Hilbert space (algebraic-topological concept) and probabilities (statistical concept). However, it is necessary to describe how the Quantum Mechanics "see" the world, on other words, how the Quantum theory and mechanisms could represents (and interprets) the nature.

Postulate 2.1: Mechanical Aspect

Every dynamical variable (physical concept) there corresponds a linear operator (mathematical object), and the possible values of the dynamical variable are the eigenvalues of the operator.

Now, it is possible to see a directly connection between the last chapter and the physical contents. Although, in CM the physical reality is a well define concept, i.e. in any instant we can look at a car a obtain their velocity and position, moreover, a priori, the formalism permits (via Euler-Lagrange equation) to determine the evolution e contra-evolution of all elements. On the other hand, due to the complementary principle, it is impossible in QM. The final remark: in QM we lost the "human intuition". Our world is a classical one! It a lot weird to think that the physical reality elements are linear operators acting in an abstract and infinity vector space, and their possible values as determined by a eigenvalue evaluation...

Statistical Aspect

Other important aspect of a physical theory is their methods to obtain the results of measurements, for instance, the energy levels of a atom. To illustrate the statistical emergence in QM we shall see how to describe a scattering experiment.

Let us start with some assumptions on the laboratory preparation: a preparation consists of acceleration and collimation in the apparatus shown in (CITAR FIGURA). A single measurement consists in the detection of the particle and hence the determination of the angle of scatter, θ. The experiment can be repeated with a equivalent preparation such that, in the end day, we have a set θ which represents different experimental runs. To treat this problem, we usually use a statistical approach. A statistical experiment consists of a long sequence of identical preparations and measurements. By some analysis we can provide a table of relative frequencies of the various possible outcomes. Furthermore, the connection between the relative frequencies and the probabilities holds, then, make sense talking about QM.

The experimental procedure can be viewed as a combination of two process

1. Preparation: in our scattering experiment the preparation consists of passing a particle through the acceleration. On other words, a preparation determines the elements of the output set and their probabilities.

2. Measurement: a measure returns one possible value of the output set. In the scattering experiment in question, the measurement consists of the detection of the particle in a angle in relation to a fixed point.

Before we going forward, let us make some important remark: Let O be an object, then, with some external interaction (e.g., experimental procedure), O

can be prepared. Thus, the probability distribution of the possible outcomes are fully determined, but we do not nothing about it (because we do not have measure). Moreover, note that the preparation concept is simple but has some particularities, in special, two distinct preparation can given the same distribution, for example, the eigenstates of σ_x and σ_y have $1/2$ of a measure of σ_z yields positive (or negative). Another observation: two identical objects, each subjected to an identical preparation, may behave differently in the subsequent measurements.

Since a preparation is independent of the specific measurement that may follow it, the preparation must determine probability distribution for all such possible measurements, and the result of this is a definition of a state. A state is identified as the specification of a probability distribution for any observable. In other point of view, to obtain the probability distribution of the outcomes it is necessary the knowledge over the observable (which you will measure) and the state (preparation).

We seen that, in general, a physical theory has a set of mathematical tools and methods to obtain their aim. Then, you can ask: in Quantum scenario, how can we evaluate the probability distribution of a set $\{\text{state } + \text{ observable}\}$? To answer this question, we have to define some statistical aspect (connection) between QM and experimental reality.

Postulate 2.2: Statistical Postulate

To each state corresponds a unique state operator. The average value of a dynamical variable R, represented by the operator R, in the virtual ensemble of events that may result from a preparation procedure for the state, represented by the operator ρ, is

$$\langle R \rangle := \frac{\mathrm{Tr}(\rho R)}{\mathrm{Tr}\,\rho},$$

where $\mathrm{Tr}(\cdot)$ denotes the trace operator.

2.1.1 Conditions on Operators

The postulate 1 said "$[\cdots]$ the possible values of the dynamical variable are the eigenvalues". Then, in their eigenbasis, ρ can be written as a diagonal of their eigenvalues. Therefore, imposing a conventional normalization, we obtain:

$$\mathrm{Tr}(\rho) = 1. \tag{2.1}$$

Consider an observable O that represents a physical quantity $\mathcal{O}$. Then, the mean value of O have to satisfied

$$\begin{aligned}
\mathrm{Tr}(\rho O) &= \mathrm{Tr}\left(\rho \sum_{i=1}^{d} o_i \left|O_i\middle\rangle\!\middle\langle O_i\right|\right) \\
&= \sum_{i=1}^{d} o_i \,\mathrm{Tr}\left(\rho \left|O_i\middle\rangle\!\middle\langle O_i\right|\right) \\
&= \sum_{i=1}^{d} o_i \,\mathrm{Tr}\left(\rho \left|O_i\middle\rangle\!\middle\langle O_i\right|\right) \\
&= \sum_{i=1}^{d} o_i \left\langle O_i\middle|\rho\middle|O_i\right\rangle,
\end{aligned}$$

where we used the spectral decomposition of O. Moreover, due to the Theorem 1.6, we have

$$\rho^\dagger = \rho. \tag{2.2}$$

However, the attentive reader must ask to yourself "any physical operators could be decomposed into the spectral decomposition?". To answer this question it is necessary build up an isomorphism $\rho \cong |\psi\rangle$. In this context, we define:

$$\rho := \left|\psi\middle\rangle\!\middle\langle\psi\right|, \tag{2.3}$$

where $|\psi\rangle$ is a normalized Dirac's vector. Such that ρ is a Hermitian operator with unitary trace. Now, returning to the decomposition of a generic physical observable, due to the above definition of state, we get

$$O^\dagger = O. \tag{2.4}$$

This scenario implies a strengthened version of Postulate 2.1:

Postulate 2.3: Physical Observable of QM

To each dynamical variable there is a hermitian operator whose eigenvalues are the possible values of the dynamical variable.

Furthermore, the average of a variable that takes on only *nonnegative operator* must itself be nonnegative. Hence,

$$\langle\psi|\rho|\psi\rangle \geqslant 0. \qquad \forall\, |\psi\rangle \tag{2.5}$$

Then, the second postulate could be viewed as

Postulate 2.4: Physical State in QM

To each state there corresponds a unique state operator, which must be Hermitian, nonnegative, and of unit trace.

2.2 General States and Pure States

In the last section was shown that $\rho \cong |\psi\rangle$ describes a *real* state. Then,

1. $\mathrm{Tr}(\rho) = 1$;
2. $\rho^\dagger = \rho$;
3. $\langle i|\rho|i\rangle$ for all $|i\rangle$ an unitary nomalized Dirac's vector.

A convex combination of Quantum states can be written as follows[4]

$$\rho := {}_i\lambda_i\rho_i, \tag{2.6}$$

[4]The convex combination say that $\sum\limits_i \lambda_i = 1$.

where $\rho_i := |\psi_i\rangle\langle\psi_i|$ such that ρ_i satisfy the above enumerated conditions. It is easy to see that ρ can also describes a Quantum state.[5]

Proof. To prove that ρ can describe a Quantum acceptable state we must verify the conditions showed in the preceding section. Firstly,

$$\mathrm{Tr}(\rho) = \sum_n \mathrm{Tr}(\rho_i) = 1.$$

Proving the unity of trace.

In terms of the Hermitian conjugation of ρ, we have

$$\rho^\dagger = \sum_i \lambda_i^* \rho_i^\dagger = \sum_i \lambda_i \rho_i = \rho.$$

Which confirms the second criterion.

Finally, due to the $\{\lambda_i\}$ are positive numbers, is easily to see that $\rho_i \geq 0$ implies that $\rho \geq 0$. □

Exercise 2.1: Matrix Form of Mean Value

Rewritten

$$\langle R\rangle = \mathrm{Tr}(|\psi\rangle\langle\psi|\, R),$$

in matrix form.

Exercise 2.2: Mathematical Conditions

Let be $M \doteq \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$. Show that M can not describe a quantum state.

Exercise 2.3: Cyclic Propriety of Trace

Show that $\mathrm{Tr}(|u\rangle\langle v|)$ holds for any pair $|u\rangle, |v\rangle$.

[5]This results prove that the set of Quantum states is a convex set. The convexity of Quantum state has a gamma of important application, for instance in Quantum Information Theory and Quantum Computation. For more details see [5].

Exercise 2.4: Quantum State Representation I

Let ρ_1 and ρ_2 be possibles representations of quantum states.

$$\rho_1 \doteq \begin{pmatrix} 1/4 & 3/4 \\ 3/4 & 3/4 \end{pmatrix} \qquad \rho_2 \doteq \begin{pmatrix} 9/25 & 12/25 \\ 12/25 & 16/25 \end{pmatrix}$$

In this scenario, which of the above matrices could represents a quantum state?

Exercise 2.5: Quantum State Representation II

Let be

$$\rho_3 = \tfrac{1}{3} |u\rangle\langle u| + \frac{2}{3} |v\rangle\langle v| + \frac{\sqrt{2}}{3} |u\rangle\langle v| + \frac{\sqrt{2}}{3} |v\rangle\langle u| .$$

Then:

1. give the matrix form of $[\rho_3]_{|u\rangle,|v\rangle}$;
2. ρ_3 can represents a quantum state?

Exercise 2.6: Quantum State Representation III

Knowing that

$$\rho_4 \doteq \begin{pmatrix} 1/2 & 0 & 1/4 \\ 0 & 1/2 & 0 \\ 1/4 & 0 & 0 \end{pmatrix} \qquad \rho_5 \doteq \begin{pmatrix} 1/2 & 0 & 1/4 \\ 0 & 1/4 & 0 \\ 1/4 & 0 & 1/4 \end{pmatrix}.$$

which of the above states are *mixed* quantum states.

Exercise 2.7: Non-Hermiticity and Complex Eigenvalues

Let $M = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$ be a matrix

1. Show that the non-Hermitian matrix M has only real eigenvalues, but its eigenvectors do not form a complete set.

2. Being non-Hermitian, this matrix must violate the conditions of (cite the theorem). Find a vector $|v\rangle$ such that $\langle v|M|v\rangle$ in complex.

Exercise 2.8: Cyclic Property of Trace

Show that $\mathrm{Tr}(AB) = \mathrm{Tr}(BA)$; and, more generally, that the trace of a product of several operators is invariant under cyclic permutation of those operators, $\mathrm{Tr}(ABC \cdots Z) = \mathrm{Tr}(ZAB \cdots)$

Exercise 2.9: Nonnegativeness

The nonnegativeness property of a general state operator ρ implies that $\mathrm{Tr}\,\rho^2 \leqslant 1$, as was shown in the course. Show, conversely, that the condition $\mathrm{Tr}\,\rho^2 \leqslant 1$, implies that ρ in nonnegative when ρ is 2×2 matrix. Show that these condition are not sufficient to ensure nonnegativeness oh ρ if its dimensions are 3×2 or larger.

Exercise 2.10: Differences Between States

Consider a dynamical variable σ that can take only two values $\{\pm 1\}$. The eigenvectors of the corresponding operator are denoted as $\{|\pm\rangle\}$. Now, consider the following states: $|\theta\rangle = \frac{1}{\sqrt{2}}\left(|+\rangle + \exp(i\theta)\,|-\rangle\right)$ and $\rho = \frac{1}{2}\left(|+\rangle\langle+| + |-\rangle\langle-|\right)$. Show that $\langle\sigma\rangle = 0$ for all of these states. What, if any, are the physical differences between these various states, and how could they be measured?

Exercise 2.11: A Measure of Spin-y

Let $\sigma_y = \begin{pmatrix} 0 & -i \\ +i & 0 \end{pmatrix}$ corresponds to a component of the spin of an electron, in units of $\hbar/2$. For a state represented by the vector $|\Psi\rangle = (\alpha, \beta)^{\intercal}$, where $\{\alpha, \beta\}$ are complex numbers, calculate the probability that the spin component is positive.

Exercise 2.12: Measurement of An Operator

Suppose that the operator

$$M \doteq \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix},$$

represents a dynamical variable. Calculate the probability $P_r(M = 0|\rho)$ for the following state operators:

1. $\rho \doteq \begin{pmatrix} 1/2 & 0 & 0 \\ 0 & 1/4 & 0 \\ 0 & 0 & 1/4 \end{pmatrix};$

2. $\rho \doteq \begin{pmatrix} 1/2 & 0 & 1/2 \\ 0 & 0 & 0 \\ 1/2 & 0 & 1/2 \end{pmatrix};$

3. $\rho \doteq \begin{pmatrix} 1/2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1/2 \end{pmatrix}.$

Exercise 2.13: Mean Value

Let $R =$ represent a dynamical variable, and $|\Psi\rangle = (a, b)^\intercal$ be an arbitrary state vector. Calculate $\left\langle R^2 \right\rangle$ in two ways:

1. Evaluate $\left\langle R^2 \right\rangle = \langle\Psi|R^2|\Psi\rangle$ directly.
2. Find the eigenvalues and eigenvectors of R,

$$R\left|r_n\right\rangle = r_n\left|r_n\right\rangle,$$

expand the state vector as a linear combination of the eigenvectors,

$$|\Psi\rangle = c_1\left|r_1\right\rangle + c_2\left|r_2\right\rangle,$$

and evaluate $\left\langle R^2 \right\rangle = r_1^2|c_1|^2 + c_2|c_2|^2$.

Exercise 2.14: Decomposition of a Quantum State

Any nonpure state operator can be decomposed into a mixture of pure states in at least two ways. Show that this can be done in infinitely many ways.

2.3 Solution

In this section we provide the solutions of the exercises of previous chapter.

2.3.1 Exercise 2.1

Any vector $|\psi\rangle$ can be represented as $|\psi\rangle = (u_1, \cdots, n)^\intercal$ in $\{|ui\rangle\}_{i=1,\cdots,n}$ basis. Then,

$$\langle R\rangle \doteq (u_1^*, \cdots, u_n^*)\,[R]_{ij}\,(u_1, \cdots, u_n)^\intercal \qquad \forall\,|\psi\rangle\,.$$

2.3.2 Exercise 2.2

The matrix M can be not represented as a quantum state.

Proof. By a directly evaluation, we have:

$$\mathrm{Tr}(M) = 2 \neq 1.$$

Then, M can not described a quantum state. □

2.3.3 Exercise 2.3

Proof. At any basis $\{|i\rangle\}$, the ket's $\{|u\rangle, |v\rangle\}$ can be decomposed as follows

$$\begin{cases} |u\rangle = \sum_i c_i\,|i\rangle\,; \\ |v\rangle = \sum_i d_i\,|i\rangle\,. \end{cases}$$

Then,

$$\begin{aligned}\mathrm{Tr}(|u\rangle\langle v|) &= \sum_i \langle i|\left(\sum_j c_j\,|j\rangle\right)\left(\sum_k d_k^*\,\langle k|\right)|i\rangle \\ &= \sum_{i,j,k} d_k^* c_j\,\langle i|j\rangle\langle k|i\rangle \\ &= \sum_i d_i^* c_i \\ &= \langle v|u\rangle\,.\end{aligned}$$

□

2.3.4 Exercise 2.4

The operator ρ_1, due to the semi-positive criterion, can not describe a quantum system, however, ρ_2 does.

Proof. To prove that ρ_1 can not describe a quantum system, we evaluate

$$\det(\rho_1 - \lambda \mathbb{1}_2) = (\lambda_1 - \lambda)(\lambda_2 - \lambda),$$

where $\{\lambda_i\}_{i=1,2}$ denotes the eigenvalues of ρ_1 and λ is a variable in domain of $P(\lambda)$ (the characteristic polynomial of ρ_1). Thus, for $\lambda = 0$ we obtain that

$$\det(\rho_1) = \lambda_1\lambda_2,$$

therefore,

$$-\frac{3}{8} = \lambda_1\lambda_2$$

which implies that one eigenvalue is negative, so ρ_1 is not positive operator.

Now, in terms of ρ_2, by a directly computation of eigenvalues, we obtain:

$$\lambda_1 = 0, \quad \lambda_2 = 1,$$

therefore, $\langle\psi|\rho_2|\psi\rangle \geqslant 0$ for all $|\psi\rangle$. Moreover, it is simple to see that $\mathrm{Tr}(\rho_2) = 1$ and $\rho_2 = \rho_2^\dagger$. Then, ρ_2 represents a quantum state. $\square$

2.3.5 Exercise 2.5

On the first item:

The matrix representation of ρ_3 in $\{|u\rangle, |v\rangle\}$ basis is given by

$$\rho_3 \doteq \begin{pmatrix} 1/3 & \sqrt{2}/3 \\ \sqrt{2}/3 & 2/3 \end{pmatrix}.$$

In terms of a quantum representation proprieties of ρ_3 : it is simple to see that $\rho_3 = \rho_3^\dagger$ (hermitian); ρ_3 has a unitary trace; and it is an positive operator

$$\begin{aligned}
\langle\psi|\rho_3|\psi\rangle =& \left(\sum_i c_i^* \langle i|\right) \left(\tfrac{1}{3}|u\rangle\langle u| + \frac{2}{3}|v\rangle\langle v| + \frac{\sqrt{2}}{3}|u\rangle\langle v| + \frac{\sqrt{2}}{3}|v\rangle\langle u|\right) \left(\sum_j c_j |j\rangle\right) \\
=& \sum_{i,j} c_i^* c_j \left[\frac{1}{3}\langle i|u\rangle\langle u|j\rangle + \frac{2}{3}\langle i|v\rangle\langle v|j\rangle \frac{\sqrt{2}}{3}\left(\langle i|u\rangle\langle v|j\rangle + \langle i|v\rangle\langle u|j\rangle\right)\right] \\
=& \sum_i \frac{|c_i|^2}{3}\left(1 + 2 + 2\sqrt{2}\right) \\
\geqslant& 0.
\end{aligned} \tag{2.7}$$

Thus, ρ_3 represents a quantum state.

2.3.6 Exercise 2.6

The operator ρ_4, due to the negativeness, do not describes a quantum state. However, ρ_5 represents a non-pure quantum state.

Proof. The relationship between the determinant and the eigenvalues of a square matrix, we have

$$\det(\rho_4) = \Pi_{i=1}^3 \lambda_i,$$

where λ_i is the i-th eigenvalue of operator ρ_4. Thus, due to

$$\det(\rho_4) = -\frac{1}{32},$$

which implies that ρ_4, at least, has a negative eigenvalues. Therefore, ρ_4 can not describe a quantum state.

For the last preposition, it is clear that $\rho_5 = \rho_5^\dagger$ (hermitian) and $\mathrm{Tr}\,\rho_5 = 1$. Furthermore, evaluating the associated eigenvalues, we obtain

$$\rho_5 = \frac{3+\sqrt{5}}{8}|u_1\rangle\langle u_1| + \frac{1}{4}|u_2\rangle\langle u_2| + \frac{3-\sqrt{5}}{8}|u_3\rangle\langle u_3|,$$

where $\{|u_i\rangle\}_{i=1,2,3}$ are the eigenkets associated[6]. However, in terms of the purity, we shall see that

$$\begin{aligned}\operatorname{Tr}\rho_5^2 \doteq& \operatorname{Tr}\begin{pmatrix} 1/4 & 0 & 1/16 \\ 0 & 1/16 & 0 \\ 1/16 & 0 & 1/16 \end{pmatrix} \\ =& \frac{3}{8} \\ <& 1 \end{aligned}$$

□

2.3.7 Exercise 2.7

Item (A):

Evaluating the eigenvalues of M, we obtain: $\lambda = 1$ with algebraic multiplicity equals two. In terms of this eigenvalue we compute the eigenvectors as follows

$$\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \implies b = 0;$$

Therefore, the unique eigenvector is given by $|+\rangle \doteq (1,0)^\intercal$. In this sense, we shall verify that the eigenbasis of M-operator can not span any vector in $\mathcal{H}$, then, it is not a complete set.

Item(B):

let $|v\rangle = \sum_i c_j |i\rangle$ represents a generic vector acting in $\mathcal{H}$, we can compute any matrix element via

$$\langle v|M|v\rangle \doteq \begin{pmatrix} c_1^* & c_2^* \end{pmatrix}\begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} |c_1|^2 + |c_2|^2 + c_1^* c_2 \end{pmatrix}.$$

Moreover, due to the complex decomposition into reals, we have $c_i = a_i + ib_i$ ($i = 1, 2$):

$$\langle v|M|v\rangle = a_1^2 + a_2^2 + b_1^2 + b_2^2 + a_1a_2 + b_1b_2 + i(a_1b_2 - b_1a_2),$$

such that M_{ij} is a complex number, in general.

[6]Their forms are not relevant, only the semi-definiteness implies for the spectral decomposition.

2.3.8 Exercise 2.8

Proof. To prove this propriety, first we shall to consider a follow sentence: a finite composition of linear operators is a linear operator:

Proof. Let $T_t = BC \cdots Z$ be a finite composition of linear operators, then, for any linear combination of $\{c_i; |i\rangle\}$

$$\begin{aligned} T_t \left(\sum_i c_i \, |i\rangle \right) =& BC \cdots Y \left(\sum_i c_i Z \, |i\rangle \right) \\ =& \sum_i c_i \left(BC \cdots YZ \right) (|i\rangle), \end{aligned}$$

where we use that the set $\{$*Letter*$\}$ are linear. □

Therefore, it is only necessary to prove the cyclic propriety of trace for two different operators (e.g., A, T_t). To do this, we compute:

$$\begin{aligned} \mathrm{Tr}\left(AT_t\right) &= \sum_i \langle i| \, AT_t \, |i\rangle \\ &= \sum_{ij} A_{ij} T_{t_{ji}} \end{aligned}$$

However, $\omega_{\mu\nu}\tau^{\mu\nu}$ is a scalar, in this sense we can rewritten the above equation as follows

$$\begin{aligned} \mathrm{Tr}\left(AT_t\right) &= \sum_i \langle i| \, AT_t \, |i\rangle \\ &= \sum_{ij} T_{t_{ji}} A_{ij} \\ &= \sum_j \, \langle j|T_t A|j\rangle \\ &= \mathrm{Tr}(T_t A). \end{aligned}$$

□

2.3.9 Exercise 2.9

if ρ describes a quantum state, then

$$\begin{cases} \sum_n \rho_{nn} = 1 \\ \sum_n \rho_{nn}^2 \leqslant 1 \end{cases} \implies \sum_n \rho_{nn}^2 \leqslant \left(\sum_n \rho_{nn} \right)^2 .$$

For n equals two, we have

$$\rho_{11}\rho_{22} \geqslant 0,$$

which implies that ρ_{11} and ρ_{22} have the same sign. However, because of the unitary trace, it is verified that we cannot have ρ_{11} and ρ_{22} both negative. Thus, the density matrix ρ is positive semi-define.

For a generic $n \geqslant 2$

$$\left(\sum_{i=1} \rho_{ii} \right)^2 = \left(\sum_{i=1} \rho_{ii} \right) \left(\sum_{j=1} \rho_{jj} \right) = \sum_{i=1} \rho_{ii}^2 + 2 \sum_{i=1} \sum_{\substack{j=1 \\ j \neq i}} \rho_{ii}\rho_{jj},$$

hence,

$$\sum_{i=1} \sum_{\substack{j=1 \\ j \neq i}} \rho_{ii}\rho_{jj} \geqslant 0.$$

Note that is impossible to reply the discussion on above paragraph. Thus, it is clear that the condition $\operatorname{Tr} \rho^2$. is necessary but not sufficient for $n \geqslant 3$.

2.3.10 Exercise 2.10

First of all, we have to compute the mean value of σ_z in $|\theta\rangle$ and ρ.

$$\begin{aligned} \langle \sigma_z \rangle_{|\theta\rangle} \equiv \langle \sigma_z \rangle_\theta =& \langle \theta | \sigma_z | \theta \rangle \\ =& \frac{1}{2} \left(\langle + | + \exp(-i\theta) \langle - | \right) \left(|+\rangle\langle+| - |-\rangle\langle-| \right) \left(|+\rangle + \exp(i\theta) |-\rangle \right) \\ =& 0. \end{aligned}$$

Providing that θ state has a null mean value of spin-z. Moreover, For a ρ density, we obtain

$$\begin{aligned}\langle\sigma_z\rangle_\rho &= \mathrm{Tr}\left[\frac{1}{2}(|+\rangle\langle+| + |-\rangle\langle-|)(|+\rangle\langle+| - |-\rangle\langle-|)\right]\\ &=0.\end{aligned}$$

Hence, both states ρ and $|\theta\rangle$ have the same mean value for σ_z.

Now, we shall to consider a measurement of an orthogonal direction of spin, for instance σ_x. The σ_x has the following eigenvalues equations

$$\sigma_x |\pm\rangle_x = \pm |\pm\rangle_x ,$$

where $|\pm\rangle = \frac{1}{\sqrt{2}}(|+\rangle \pm |-\rangle)$. In terms of this non-commuting (in relation to σ_z) we could performing a measure and obtain a substantial difference between a mixed and a pure state. To evaluate the last preposition, we have to rewritten $\{|\theta\rangle, \rho\}$ in terms of x-basis:

$$\begin{aligned}|\theta\rangle_x =&\frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}(|+\rangle_x + |-\rangle_x) + \exp(i\theta)\frac{1}{\sqrt{2}}(|+\rangle_x - |-\rangle_x)\right)\\ &= \exp(i\theta/2)\left[\frac{\exp(-i\theta/2)+\exp(i\theta/2)}{2}|+\rangle_x + \frac{\exp(-i\theta/2)-\exp(i\theta/2)}{2}|-\rangle_x\right]\\ &= \exp(i\theta/2)\left[\cos(\theta/2)|+\rangle_x - i\sin(\theta/2)|-\rangle_x\right]\\ \rho =&\frac{1}{2}(|+\rangle\langle+|_x + |-\rangle\langle-|_x).\end{aligned}$$

Therefore, the mean value of σ_x in θ-state and ρ:

$$\begin{aligned}\langle\sigma_x\rangle_\theta &= (\cos(\theta/2)\langle+|_x + i\sin(\theta/2)\langle-|_x)(|+\rangle\langle+|_x - |-\rangle\langle-|_x)(\cos(\theta/2)|+\rangle_x - i\sin(\theta/2)|-\rangle_x)\\ &= \cos^2(\theta)\\ \langle\sigma_x\rangle_\rho &=0.\end{aligned}$$

Hence, different states given a different measure of a quantum observable (spin-x) and, due to the Copenhagen's interpretation of QM, two states are equal if and only if they give the same measurements results for any observable.

2.3.11 Exercise 2.11

If Ψ are represented by α, β components in spin-z basis. Then, in spin-y canonical basis it is assume the following form:

$$
\begin{aligned}
|\Psi\rangle =& \alpha\left(\frac{|+\rangle_y + i\,|-\rangle_y}{\sqrt{2}}\right) + \beta\left(\frac{|+\rangle_y - i\,|-\rangle_y}{\sqrt{2}}\right) \\
=& \left(\frac{\alpha+\beta}{\sqrt{2}}\,|+\rangle_y\right) + i\left(\frac{\alpha-\beta}{\sqrt{2}}\right)|-\rangle_y\,.
\end{aligned}
$$

In this scenario, the probability to obtain $+1$ in a measure of σ_y is given by:

$$
P_r\left(\sigma_y = +1|\,|\psi\rangle\right) = \left|\frac{\alpha+\beta}{2}\right|^2 = \frac{1}{2}\left(|\alpha|^2 + |\beta|^2 + 2\,\mathrm{Re}\{\alpha\beta\}\right).
$$

2.3.12 Exercise 2.12

Diagonalizing the M matrix, we obtain the following eigenvalue:

$$
\lambda_1 = 0; \quad \lambda_2 = \sqrt{2}; \quad \lambda_3 = -\sqrt{2}.
$$

Moreover, it is possible to determine the eigenvector associate with $\lambda = 0$ measure. The result of this process can be viewed as following

$$
|\lambda_0\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle - |2\rangle\right).
$$

Hence, the matrix representation of M_0 projector (projector associated with output $M = 0$) in the $\{|0\rangle, |1\rangle, |2\rangle\}$ basis is

$$
\begin{pmatrix}
1/2 & 0 & -1/2 \\
0 & 0 & 0 \\
-1/2 & 0 & 1/2
\end{pmatrix}.
$$

Thus, it is easy to obtain the probabilities to obtain $M = 0$ in a measure of M for any state, for example:

$$
P_r(0|\psi_1) = 3/8 \quad P_r(0|\psi_2) = 0 \quad P_r(0|\psi_3) = 1/2.
$$

2.3.13 Exercise 2.13

To answer the first item, we compute:

$$\begin{aligned}\left\langle R^2\right\rangle_\psi =&\begin{pmatrix} a^* & b^* \end{pmatrix}\begin{pmatrix} 40 & -30 \\ -30 & 85 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix}\\ =&a^*(40a-30b)+b^*(-30a+85b)\\ =&40|a|^2+85|b|^2-60\,\mathrm{Re}\{ab\}\end{aligned}$$

Now, in terms of the second item, we evaluate the eigenvalues, r_n $(n = 1,2)$ of R:

$$r_1 = 10; \quad r_2 = 5.$$

The associated eigenvectors (normalized) are defined as follows

$$|r_1\rangle = \frac{1}{\sqrt{5}}(-|0\rangle + 2|1\rangle); \quad |r_2\rangle = \frac{1}{\sqrt{5}}(2|0\rangle + |1\rangle).$$

Then, if $|\psi\rangle = \sum_{i=1}^{2} c_i |r_i\rangle$, we obtain:

$$|\psi\rangle = \left(\frac{2b-a}{\sqrt{5}}\right)|r_1\rangle + \left(\frac{2a+b}{\sqrt{5}}\right)|r_2\rangle,$$

and

$$\begin{aligned}\left\langle R^2\right\rangle_\psi =&r_1^2|c_1|^2+r_2^2|c_2|^2\\ =&(100)^2\frac{(2b^*-a^*)(2b-a)}{5}+(5)^2\frac{(2a^*+b^*)(2a+b)}{5}\\ =&20(4|b|^2+|a|^2-2(b^*a+a^*b))+5(4|a|^2+|b|^2+2(a^*b+b^*a))\\ =&85|b|^2+40|a|^2-60\,\mathrm{Re}\{ab\}.\end{aligned}$$

Which re-obtain the previous result.

2.3.14 Exercise 2.14

3 Kinematics and Dynamics

In the preceding chapters, we established the formal foundation of Quantum Mechanics (QM). In this chapter, we will explore how the symmetries of space-time can elegantly provide a bridge between this abstract formalism and the physical reality, specifically the equations of motion and the connection between physical quantities and Hermitian operators.

3.1 Transformations of States and Observable

Operations as displacements, rotations and transformations between frames are elements of space-time transformations. The application of space-time transformations in observables and states given a fundamental tool to obtain new observables (and states). However, certain relations must be preserved by these transformations.

Firstly, let $\mathcal{A}$ be a physical quantity and the operators A and A' their operators description in two distinct referential frames S and S', respectively. Then, via the mechanical postulate, the eigenvalues, a_i of A (or A') are the possible outputs of a measurement of A. Hence, a_i must be invariant under space-time transformation.

The second invariant quantity is the norm of a vector. Let $|\psi\rangle$ be a a vector, then $\left|\left\langle\phi'_n|\psi'\right\rangle\right|^2 \equiv |\langle\phi_n|\psi\rangle|^2$.

The mathematical characterization of these transformations is clarified by the following theorem:

Theorem 3.1: Wigner's Theorem

Any mapping of the vector space onto itself that preserves the value of $|\langle\phi|\psi\rangle|$ may be implemented by an operator U:

$$|\psi\rangle \longrightarrow |\psi'\rangle = U\,|\psi\rangle\,;$$
$$|\phi\rangle \longrightarrow |\phi'\rangle = U\,|\phi\rangle\,,$$

with U being either unitary (linear) or antiunitary (antilinear).

For instance: if U is unitary, then by definition of $UU^\dagger = U^\dagger U = \mathbb{1}_d$, where the right side operator is the identity. Thus $\left\langle\phi'|\psi'\right\rangle = \langle\phi|\psi\rangle$. On other hand, if U is antiunitary, then $U(c\,|v\rangle) = c^* U(|v\rangle)$, which implies that $\left\langle\phi'|\psi'\right\rangle = (\langle\phi|\psi\rangle)^*$.

The observables transformations must let invariant the eigenvalues of a such operator:

$$A'[U(|\phi\rangle_n)] = a_n(|\phi\rangle_n) \implies (U^{-1}AU)\,|\phi\rangle_n = a_n\,|\phi\rangle_n\,. \tag{3.1}$$

Hence, the desired transformation of operators is a similarity transformation $A \longrightarrow A' = UAU^{-1}$.

Let consider a family of unitary operators $U(\tau)$, that depend on single continuous parameter τ. $U(\tau)$ is such that $U(0) \equiv \mathbb{1}_d$ be the identity operator, and let $U(\tau_1+\tau_2) \equiv U(\tau_1)U(\tau_2)$. In that scenario, $U(\tau)$ can be viewed as a element of a group.

If $U(\tau)$ is a smooth function, using the Taylor expansion around $\tau = 0$ we obtain:

$$U(\tau) = \mathbb{1}_d + \tau \left.\frac{\mathrm{d}U}{\mathrm{d}\tau}\right|_{\tau=0} + \mathcal{O}(\tau^2),$$

or, via unitary condition

$$UU^\dagger = \mathbb{1}_d + \tau\left[\frac{\mathrm{d}U}{\mathrm{d}\tau} + \frac{\mathrm{d}U^\dagger}{\mathrm{d}\tau}\right]\Bigg|_{\tau=0} + \mathcal{O}(\tau^2).$$

Hence,

$$\frac{\mathrm{d}U}{\mathrm{d}\tau} = iK \quad (K^\dagger = K), \tag{3.2}$$

with K is generator of the family of unitary operators $\{U(\tau)\}$. Moreover, due to composition rule satisfied for U, we obtain: $U(\tau_1+\tau_2) = U(\tau_1)U(\tau_2)$. The above equation can be establishes the following form:

$$\begin{aligned}\frac{\mathrm{d}U}{\mathrm{d}\tau} =& \frac{\mathrm{d}}{\mathrm{d}\tau}\left[U(\tau-\tau_2)U(\tau-\tau_1)\right]\\ =& U(s_2)\frac{\mathrm{d}U(s_1)}{\mathrm{d}s_1} + U(s_1)\frac{\mathrm{d}U(s_2)}{\mathrm{d}s_2},\end{aligned}$$

where we used $s_i := \tau - \tau_i \quad (i=1,2)$. Therefore, in the point $\tau = \tau_2$, we have

$$\frac{\mathrm{d}U}{\mathrm{d}\tau}\Big|_{\tau=\tau_2} = U(\tau_2)iK.$$

This first order ODE under $U(0) = \mathbb{1}_d$ has the solution

$$U(\tau) := \exp(iK). \tag{3.3}$$

In general, each continuous symmetry can be viewed as a element of a lie group. A lie group, $\mathcal{G}$, is a group such that, given an element $\epsilon^\alpha \in \mathcal{G}$, then exist $R(g)$ defined as follows

$$R(g) := \exp(i\epsilon^\alpha K_\alpha),$$

where K_α is the generator of the symmetry associated to ϵ^α, and $R(g)$ is the mapping between the lie-algebra's element and their representation (unitary). In special, can be proven that every element g admits a unitary representation $R(g)$., see (REF DE TEO. DE GRUPOS).

3.2 The symmetries of Space-Time

The symmetries of space-time (ST) are rotations, displacements (spacial or temporal), and transformations between uniformly moving references frames. In a context where we only restrict ours systems to a non-relativistic one $(v \ll c \equiv 1)$ the set of all such transformations is written as follows[1]

$$x^i \longrightarrow x^{i'} = R(x^i) + a^i + v^i x^0; \tag{3.4a}$$

$$x^0 \longrightarrow x^{0'} = x^0 + s. \tag{3.4b}$$

Here $R : \mathbb{R}^3 \mapsto \mathbb{R}^3$ describes a rotation operation, a^i is a space displacement, v^i is the velocity of a moving referential, and s is a temporal displacement.

let $\tau_k := \tau_k(s_k; R_k, a^i_k, v^i_k)$ denote such a transformation. Then due to the space-time transformations (STT) form a group, the composition $\tau_3 = \tau_2\tau_1$ are defined as follows:

$$\begin{aligned}
\tau_1(x^\mu) \equiv x^\mu_1 &= \left(x^0 + s_1; R_1(x^i) + a^i_1 + v^i_1 x^0\right) \\
x^\mu_2 \equiv \tau_2(x^\mu_1) &= \left(x^0 + s_1 + s_2; R_2(R_1(x^i) + a^i_1 + v^i_1 x^0) + a^i_2 + v^i_2(x^0 + s_1)\right) \\
&\equiv \left(x^0 + s_3; R_3(x^\mu) + a^i_3 + v^i_3 x^0\right).
\end{aligned}$$

Hence,

$$\begin{cases}
s_3 := s_1 + s_2; \\
R_3 := R_2(R_1); \\
a^i_3 := R_2(a^i_1) + s_1 v^i_2 + a^i_2; \\
v^i_3 := R_2(v^i_1) + v^i_2.
\end{cases} \tag{3.5}$$

3.3 Generators of the Galilei Group

The Galilei group has ten possibles generators. They are: three for rotations, three for space displacements, one for time displacement, and three for uniformly referential swap. Denoting this generators by K_μ $(\mu = 0, \cdot, 9)$, and using that every STT can be viewed as a lie group element, we obtain

$$U(\tau) := \exp(is^\mu K_\mu). \tag{3.6}$$

[1]In the below pair of equations we describe how the uniformly moving frame S' (in relation to another S) see the space-time vectors defined in S sets of coordinates x^μ. For completeness, we were used the *covariant notation* where: $x^\mu := (t; x^1, x^2, x^3)$; $x_\nu := g_{\nu\mu}x^\mu$; $g_{\mu\nu} := \mathbb{1}_4$.

With s^μ denotes the ten parameters that define the $\tau = \tau(s^\mu)$. Moreover, note that we used the Einstein's convention to summation.

Now, let us take $s^\mu \to 0$, then the general infinitesimal unitary operator could be rewritten in terms of

$$U(\tau) = \mathbb{1}_{10} + is^\mu K_\mu. \tag{3.7}$$

One of the most important concept in group theory is the *commutator* (defined as follows). In this context, we define the commutator between two operators (generators) via the following argumentation

$$\begin{aligned} e^{i\varepsilon K_\mu} e^{i\varepsilon K_\nu} e^{-i\varepsilon K_\mu} e^{-i\varepsilon K_\nu} &= \left(\mathbb{1} + i\varepsilon K_\mu - \varepsilon^2 K_\mu^2\right)\left(\mathbb{1} + i\varepsilon K_\nu - \varepsilon^2 K_\nu^2\right) \\ &\quad \left(\mathbb{1} - i\varepsilon K_\mu + \varepsilon^2 K_\mu^2\right)\left(\mathbb{1} - i\varepsilon K_\nu + \varepsilon^2 K_\nu^2\right) + \mathcal{O}(\varepsilon^3) \\ &= \mathbb{1} + \varepsilon^2 \left(K_\nu K_\mu - K_\mu K_\nu\right) + \mathcal{O}(\varepsilon^3) \end{aligned} \tag{3.8}$$

Although, how the STT forms a group, the above composition can be rewritten in terms of a composition (equally was argued in the deviation of (3.7)):

$$U(\tau) = \exp(is^\mu K_\mu).$$

Otherwise, it is know that the quantum states are invariant under the action of a global phase, hence,

$$e^{i\omega} U(\tau) = \mathbb{1}_{10} + is^\mu K_\mu + i\omega \mathbb{1}_{10}, \tag{3.9}$$

has the same physical significance that $U(\tau)$.

The invariance under global phases implies that (3.8) is equal to (3.9). Symbolically, we obtain

$$\mathbb{1} + \varepsilon^2 \left(K_\nu K_\mu - K_\mu K_\nu\right) = \mathbb{1} + \varepsilon^2 \left(ic^\lambda_{\nu\mu} K_\lambda + ib_{\nu\mu}\mathbb{1}\right).$$

Which was used (without generality loss) the covariant assumptions $s^\lambda \to \varepsilon^2 c^\lambda_{\nu\mu}$ and $\omega \to \varepsilon^2 b_{\nu\mu}$. Finally, we define the commutator as following

$$[K_\mu, K_\nu] := ic^\lambda_{\mu\nu} K_\lambda + ib_{\mu\nu}\mathbb{1}, \tag{3.10}$$

for every pair of generators K_μ's. Note that, $c_{\mu\nu}^{\lambda}$ is such that satisfies the compositions rules and for $\omega = 0$ we have that $b_{\mu\nu} \to 0$.

Then then generators of STT are the elements of the set $\{-J_i, -P_i, G_i, H\}$ with $(i = 1, 2, 3)$ where they are respectively: the 3- rotations generators, the 3- space displacements generators, 3- uniformly velocity referential change, and H is the time displacement generator.

Had defined the STT generators, let us evaluate some commutators (i.e., determine the algebraic structure of the Galilei group). To do this we must use the

4 Coordinates Representation

Exercise 4.1: Invariance of SE

Prove that Schrödinger equation (SE) is invariant under Galilei's transformations

Exercise 4.2: Evaluating Probabilities flux

Consider the two above wave-equations

$$\psi(x^j) = C\exp\big(ik_j x^j\big); \qquad \psi(\mathbf{x}) = C_1\exp(i\mathbf{k_1}\cdot\mathbf{x}) + C_2\exp(i\mathbf{k_2}\cdot\mathbf{x}).$$

Show that $J_1 = \frac{|C|^2\hbar\mathbf{k}}{M}$ and $J_2 =$

Exercise 4.3: P- matrix

Obtain the explicit form of transference matrix, section 4.7 [1]. Moreover, determine the reflection and transmission coefficients

Exercise 4.4

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Exercise 4.5: Free-Particle Propagator

Show that the free particle propagator (determined via path integral formalism) is a solution o SE. Therefore, the Feymann path integral formalism is an alternative way to obtain solution in QM problems

Exercise 4.6: Commutator in coordinates Space

Show that the commutator of the momentum operator with a function of the position operator is given by $[f(x), P_x] = i\hbar\frac{\partial f}{\partial x}$.

Exercise 4.7: Eigenvalues, Eigenfunction, and a infinite potential well

Calculate the energy eigenvalues and eigenfunctions for a particle in one dimensional confined by the infinite potential well: $W(x) = 0$ for $0 < x < a$, otherwise $W(x) = \infty$. Calculate the matrices for the position and momentum operator, Q and P, using these eigenfunctions as a basis

Exercise 4.8: Toy Model: Electron - Metal

The simplest model for the potential experienced by an electron at the surface of a metal is a step:

$$W(X) = \begin{cases} -V_0 & \text{for} x < 0 \\ 0 & \text{for} x > 0 \end{cases}$$

Exercise 4.9: Inverse of r^2 Potential

For a spherical potential of the form $W(x) = C/r^2$, obtain the asymptotic form of the spherically symmetric solutions of the wave equation in the neighborhood of $r = 0$, and hence For what range of C for which they are physically admissible.

Exercise 4.10: Inverse of r^n

This problem

Exercise 4.11: Probability Flux

The probability flux $\mathbf{J}(\mathbf{x}, t)$ is not uniquely determined by the continuity, since also the continuity equation is also satisfied by $\mathbf{J}(\mathbf{x}, t) + \mathbf{f}(\mathbf{x}, t)$, where $\boldsymbol{\nabla} \cdot (\mathbf{f}) = 0$. Show that if the motion is only in one dimension this formal nonuniqueness has no effect, and so the result is practically unique in this case.

Exercise 4.12: Transmission and Reflection

Calculate the transmission and reflection coefficients for an attractive one-dimensional square well potential: $W(x) = -V_0 < 0$ for $0 < x < a$; $W(x) = 0$ otherwise. Give a qualitative explanation for the vanishing of the reflection coefficient at certain energies.

Exercise 4.13: Transfer Matrix

Use the transfer matrix method to calculate the transmission coefficient for the system of two rectangular barriers shown, for energies in the range $0 < E < V_0$.

Exercise 4.14: Delta Potential

1. Determine the condition on the state function $\psi(x)$ at the one dimensional delta function potential, $W(x) = c\delta(x)$.
2. Calculate the ground state of a particle in the one-dimensional attractive potential $W(x) = c\delta$ with $C < 0$.

Exercise 4.15: QM and Path Integrals

What is the action associated with the propagation of a free particle along the classical path from (x_1, t_1) to (x_2, t_2)? Express the Feymann phase factor in terms of the de Broglie wavelength.

Exercise 4.16: Green Function and Propagator

Show the relationship between Green Function and propragator of a free particle

Exercise 4.17: Path Integral

Path integral

4.1 solutions

4.1.1 Exercise 4.1

Yes, the Schrödinger equation is invariant under Galilei's transforms.

Proof. Let $F = F(x,t)$ be a generic function defining in terms of the space-time coordinates in a referential (here denoted as S). Moreover, F can be written in terms of another referential, denoted as S', via an application of the Galilei's space-time transformation (e.g, another referential moving uniformly, v, in relation to the first one). Symbolically , we have

$$\begin{cases} t \longrightarrow t' = t \\ x \longrightarrow x' = x + vt \end{cases} \qquad \Longrightarrow \; F(x,t) \longrightarrow F'(x',t').$$

If we consider the invariance of the probability distribution[1], then

$$\psi(x,t) = \exp(iF(x,t))\psi'(x',t'),$$

where, off course, $\psi(x,t)$ represents the probability density to find a particle in $\{x, x + \mathrm{d}x\}$.

Before we evaluate the symmetry of the ES, let us make some remarks. Note, any space-time function admits the follow differential form in S' referential

$$\begin{aligned} \mathrm{d}F =& \frac{\partial F}{\partial x'}\,\mathrm{d}x' + \frac{\partial F}{\partial t'}\,\mathrm{d}t' \\ =& \frac{\partial F}{\partial x'}\,\mathrm{d}x + \left(\frac{\partial F}{\partial x'}v + \frac{\partial F}{\partial t'}\right)\mathrm{d}t\,. \end{aligned}$$

Which implies the differential space-time transformations:

$$\begin{cases} \dfrac{\partial}{\partial x'} = \dfrac{\partial}{\partial x}; \\ \dfrac{\partial}{\partial t'} = \dfrac{\partial}{\partial t} + v\dfrac{\partial}{\partial x}. \end{cases}$$

[1]This assumptions is justified once the probability distribution only tell us about the experimental reality, in this sense, their cannot depend of the referential frame.

Now, we shall compute the Schrödinger equation (SE) in S':

$$\frac{-\hbar^2}{2m}\partial^2_{x'}\psi' + W\psi' = i\hbar\partial_{t'}\psi'$$

or, in terms of S frame

$$\frac{-\hbar^2}{2m}\partial^2_{x}\left(\exp(iF)\psi\right) + W\exp(iF)\psi = i\hbar\left[\frac{\partial}{\partial t} + v\frac{\partial}{\partial x}\right]\left(\exp(iF)\psi\right).$$

Let us evaluate term-term of the above equation

1. Spatial terms:

$$\begin{aligned}\partial_x\partial_x\left(\exp(-iF)\psi\right) =&\partial_x\left[\exp(-iF)\left(-i\frac{\partial F}{\partial x} + \frac{\partial\psi}{\partial x}\right)\right]\\ =&\exp(-iF)\left[\frac{\partial^2\psi}{\partial x^2} - 2i\frac{\partial F}{\partial x}\frac{\partial\psi}{\partial x} - \left(\left(\frac{\partial F}{\partial x}\right)^2 + i\frac{\partial^2 F}{\partial x^2}\right)\psi\right].\end{aligned}$$

2. Temporal terms:

$$\frac{\partial}{\partial t'}\left(\exp(-iF)\psi\right) = \exp(-iF)\left[\frac{\partial\psi}{\partial t} + v\frac{\partial\psi}{\partial x} - i\left(\frac{\partial F}{\partial t} + v\frac{\partial F}{\partial x}\right)\psi\right].$$

Finally, return in SE for ψ' with the above pair of expressions, we obtain

$$\begin{aligned}\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + W(x)\psi - i\hbar\frac{\partial\psi}{\partial t} =& - i\hbar\left(\frac{\hbar}{m}\frac{\partial F}{\partial x} - v\right)\frac{\partial\psi}{\partial x}\\ &- \left[\frac{\hbar^2}{2m}\left(\frac{\partial F}{\partial x}\right)^2 + \frac{i\hbar}{2m}\frac{\partial^2 F}{\partial x^2} - \hbar\frac{\partial F}{\partial t} - \hbar v\frac{\partial F}{\partial x}\right]\psi.\end{aligned}$$

Therefore, for SE be invariant under Gelilei's transforms the right side equation must be vanish for all x. In this context, we have

$$\begin{cases}\dfrac{\hbar}{m}\dfrac{\partial F}{\partial x} - v = 0\\ \dfrac{\hbar^2}{2m}\left(\dfrac{\partial F}{\partial x}\right)^2 + \dfrac{i\hbar}{2m}\dfrac{\partial^2 F}{\partial x^2} - \hbar\dfrac{\partial F}{\partial t} - \hbar v\dfrac{\partial F}{\partial x} = 0\end{cases} \implies f(x,t) = \frac{mv}{\hbar}x - \frac{mv^2}{\hbar 2}t.$$

Hence, set $F(x,t) := \dfrac{mv}{\hbar}x - \dfrac{mv^2}{2\hbar}t$ we obtain that SE is invariant, and more

$$
\begin{aligned}
\psi(x,t) &= \exp(iF)\psi'(x',t') \\
&= \exp\left[i\left(\frac{mv}{\hbar}x - \frac{mv^2}{2\hbar}t\right)\right]\psi'(x-vt,t) \\
&= \exp\left[\frac{i}{\hbar}\left(mvx - \frac{mv^2}{2}t\right)\right]\exp\left[\frac{i}{\hbar}\left(k\hbar(x-vt) - \tfrac{k^2\hbar^2}{2m}\right)\right] \\
&= \exp\left[\frac{i}{\hbar}\left(\hbar k + mv\right)x - \frac{i}{\hbar}\left(\frac{\hbar^2k^2 + \hbar kv + m^2v^2}{2m}\right)\right] \\
&= \exp\left[\frac{i}{\hbar}\left(\hbar k + mv\right)x - \frac{i}{\hbar}\frac{\left(\hbar k + mv\right)^2}{2m}\right],
\end{aligned}
$$

where we used that $\psi(x,t) = \exp\left[i(kx - \frac{k^2\hbar}{2m})\right]$ (solution for $W(X) = 0$). So the Schrödinger's wave arguments transforms as $\hbar k \longrightarrow \hbar k + mv$ which is a Galilei's invariant! $\square$

4.1.2 Exercise 4.2

For the first wave equation, we can identify $S(x.t) = \hbar\mathbf{k}\cdot\mathbf{x}$, hence,

$$\mathbf{J_1}(x,t) = \frac{|C|^2}{M}\boldsymbol{\nabla}S = \frac{|C|^2}{M}\hbar\mathbf{k}.$$

For the second case: firstly we compute

$$
\begin{aligned}
\psi^*\boldsymbol{\nabla}\psi &= \left(c_1^*\exp(-i\mathbf{k_1}\cdot\mathbf{x}) + c_2^*\exp(-i\mathbf{k_2}\cdot\mathbf{x})\right) i\left(c_1\mathbf{k_1}\exp(i\mathbf{k_1}\cdot\mathbf{x}) + c_2\mathbf{k_2}\exp(i\mathbf{k_2}\cdot\mathbf{x})\right) \\
&= i\left(|c_1|^2\mathbf{k_1} + |c_2|^2\mathbf{k_2} + \underbrace{C_1^*C_2\mathbf{k_2}\exp[i(\mathbf{k_2}-\mathbf{k_1})\cdot\mathbf{x}] + C_2^*C_1\mathbf{k_1}\exp[i(\mathbf{k_1}-\mathbf{k_2})\cdot\mathbf{x}]}_{(*)}\right).
\end{aligned}
$$

However the last two terms can also be written as

$$
\begin{aligned}
(*) =& \mathbf{k_2}[\mathrm{Re}(C_1^*C_2)\cos[(\mathbf{k_2}-\mathbf{k_1})\cdot\mathbf{x}] - \mathrm{Im}(C_1^*C_2)\sin[(\mathbf{k_2}-\mathbf{k_1})\cdot\mathbf{x}] \\
&+ i\left(\mathrm{Re}(C_1^*C_2)\sin[(\mathbf{k_2}-\mathbf{k_1})\cdot\mathbf{x}] + \mathrm{Im}(C_1^*C_2)\cos[(\mathbf{k_2}-\mathbf{k_1})\cdot\mathbf{x}]\right)] \\
&+ \mathbf{k_1}[\mathrm{Re}(C_2^*C_1)\cos[(\mathbf{k_2}-\mathbf{k_1})\cdot\mathbf{x}] + \mathrm{Im}(C_2^*C_1)\sin[(\mathbf{k_2}-\mathbf{k_1})\cdot\mathbf{x}] \\
&+ i\left(-\mathrm{Re}(C_2^*C_1)\sin[(\mathbf{k_2}-\mathbf{k_1})\cdot\mathbf{x}] + \mathrm{Im}(C_2^*C_1)\cos[(\mathbf{k_2}-\mathbf{k_1})\cdot\mathbf{x}]\right)].
\end{aligned}
$$

Finally, we shall see that

$$\begin{aligned}\mathrm{Im}(\psi^*\boldsymbol{\nabla}\psi) =&|c_1|^2\mathbf{k_1}+|c_2|^2\mathbf{k_2}+\mathrm{Re}((*))\\ =&|c_1|^2\mathbf{k_1}+|c_2|^2\mathbf{k_2}\\ &+(\mathbf{k_2}+\mathbf{k_1})[\mathrm{Re}(C_1^*C_2)\cos[(\mathbf{k_2}-\mathbf{k_1})\cdot\mathbf{x}]]\\ &-(\mathbf{k_2}+\mathbf{k_1})[\mathrm{Im}(C_1^*C_2)\sin[(\mathbf{k_2}-\mathbf{k_1})\cdot\mathbf{x}]].\end{aligned}$$

Which proves that

$$\begin{aligned}\mathbf{J_2}(x,t) =&\frac{\hbar}{m}\{|c_1|^2\mathbf{k_1}+|c_2|^2\mathbf{k_2}\\ &+(\mathbf{k_2}+\mathbf{k_1})[\mathrm{Re}(C_1^*C_2)\cos[(\mathbf{k_2}-\mathbf{k_1})\cdot\mathbf{x}]]\\ &-(\mathbf{k_2}+\mathbf{k_1})[\mathrm{Im}(C_1^*C_2)\sin[(\mathbf{k_2}-\mathbf{k_1})\cdot\mathbf{x}]]\}.\end{aligned}$$

4.1.3 Exercise 4.3

By definition, we have that:

$$P=M_1^{-1}M_2M_3^{-1}M_4, \tag{4.1}$$

where, defining $k^2=2mE/h^2$ and $\beta=2m(V_0-E)/\hbar^2$

$$M_1=\begin{pmatrix}1 & 1\\ ik & -ik\end{pmatrix}; \qquad M_2=\begin{pmatrix}1 & 1\\ \beta & -\beta\end{pmatrix};$$

$$M_3=\begin{pmatrix}e^{\beta a} & e^{-\beta a}\\ \beta e^{\beta a} & -\beta e^{-\beta a}\end{pmatrix}; \qquad M_4=\begin{pmatrix}e^{ika} & e^{-ika}\\ ike^{ika} & -ike^{-ika}\end{pmatrix}.$$

First, we evaluate the inverses matrix of M_1 and M_3[2]:

$$M_1^{-1}=\begin{pmatrix}\frac{1}{2} & -\frac{i}{2k}\\ \frac{1}{2} & +\frac{i}{2k}\end{pmatrix}; \qquad M_3^{-1}=\begin{pmatrix}\frac{e^{-\beta a}}{2} & \frac{e^{-\beta a}}{2\beta}\\ \frac{e^{\beta a}}{2} & -\frac{e^{\beta a}}{2\beta}\end{pmatrix}.$$

Now, it is only hand work to obtain P-matrix:

$$P=\begin{pmatrix}e^{ika}\left[\cosh(\beta a)+\frac{i}{2}\left(\frac{\beta}{k}-\frac{k}{\beta}\right)\sinh(\beta a)\right] & \frac{i}{2}e^{-ika}\left(\frac{\beta}{k}+\frac{k}{\beta}\right)\sinh(\beta a)\\ -\frac{i}{2}e^{ika}\left(\frac{\beta}{k}+\frac{k}{\beta}\right)\sinh(\beta a) & e^{-ika}\left[\cosh(\beta a)-\frac{i}{2}\left(\frac{\beta}{k}-\frac{k}{\beta}\right)\sinh(\beta a)\right]\end{pmatrix}.$$

[2] For this was used the software *Mathematica 12* (see the attached files).

In this context, we could obtain the transmission coefficient via the following rule:

$$T = \left|\frac{1}{p_{11}}\right|^2 = \left(\cosh(\beta a) + \frac{1}{4}\left(\frac{\beta^2 - k^2}{\beta k}\right)^2 \sinh(\beta a)\right)^{-1}.$$

However,

$$\left(\frac{\beta^2 - k^2}{\beta k}\right)^2 = \frac{(V_0 - 2E)^2}{(v_0 - E)E} = \frac{V_0^2 - 4(V_0 E - E^2)}{(v_0 - E)E} = \frac{V_0^2}{E(V_0 - E)} - 1.$$

Therefore, the last equation in addition to the definition of T, we obtain:

$$T = \left[1 + \frac{V_0^2}{4E(V_0 - E)} \sinh^2(\beta a)\right]^{-1}. \tag{4.2}$$

On the other hand, for R coefficient we have

$$R = 1 - T = 1 - \left[1 + \frac{V_0^2}{4E(V_0 - E)} \sinh^2(\beta a)\right]^{-1}$$

4.1.4 Exercise 4.4

In terms of the probability, for $x > a$ (transmitted wave), using the definition of $\mathbf{J}(x)$ we have:

$$\begin{aligned}\mathbf{J}(x > a) =& \frac{\hbar}{m} \operatorname{Im}(A_2^* \exp(-i\mathbf{k}\cdot\mathbf{x}))A_2 \exp(i\mathbf{k}\cdot\mathbf{x})) \\ =& \tfrac{|A_2|^2}{m}\hbar\mathbf{k}.\end{aligned}$$

In the case of $x < 0$ (incident wave), let us consider the following quantity

$$\begin{aligned}\psi^* \boldsymbol{\nabla}\psi =& \left(A_1^* \exp(-i\mathbf{k}\cdot\mathbf{x}) + B_1^* \exp(i\mathbf{k}\cdot\mathbf{x})\right) i\mathbf{k} \left(A_1 \exp(i\mathbf{k}\cdot\mathbf{x}) - B_1 \exp(-i\mathbf{k}\cdot\mathbf{x})\right) \\ =& i\mathbf{k}\big[|A_1|^2 - |B_1|^2 \\ & - \operatorname{Re}(A_1^* B_1)\cos(2\mathbf{k}\cdot\mathbf{x}) + \operatorname{Re}(B_1^* A_1)\cos(2\mathbf{k}\cdot\mathbf{x})\big) \\ & - \operatorname{Im}(A_1^* B_1)\sin(2\mathbf{k}\cdot\mathbf{x}) - \operatorname{Im}(B_1^* A_1)\sin(2\mathbf{k}\cdot\mathbf{x}) + i\operatorname{Im}((**))\big],\end{aligned}$$

with $(**)$ is the first line element less than $i\mathbf{k}$. Moreover, note that $\operatorname{Re}(B_1^* A_1) = \operatorname{Re}(A_1^* B_1)$ and $\operatorname{Re}(B_1^* A_1) = -\operatorname{Re}(A_1^* B_1)$, which implies that:

$$\mathbf{J}(x < 0) = \left(|A_1|^2 - |B_1|^2\right)\frac{\hbar\mathbf{k}}{m}.$$

4.1.5 Exercise 4.5

Note this exercise is a merely calculus evaluation, in this sense, we can check that via symbolic tools (mathematica). The code is attached!

4.1.6 Exercise 4.6

Proof. By assumption $f(x)$ is an analytic function of x, thus

$$f(x) = \sum_{i=1}^{\infty} a_n x^n. \tag{4.3}$$

From the above equation, we rewritten the commutator as

$$[f(x), P_x] = -\sum_{i=1}^{\infty} a_n [P_x, x^n]. \tag{4.4}$$

now, let us make some considerations on the last term of (4.4):

$$\begin{aligned}
[P_x, x^n] =& X[P_x, X^{n-1}] + [P_x, X]X^{n-1} \\
=& X\left(X[P_x, X^{n-2}] + [P_x, X]X^{n-2}\right) - i\hbar X^{n-1} \\
=& X\left[X\left(X[P_x, X^{n-3}] + [P_x, X]X^{n-3}\right)\right] - 2i\hbar X^{n-1} \\
=& X^3\left(X[P_x, X^{n-4}] - i\hbar X^{n-4}\right) - 2i\hbar X^{n-1} \\
& \vdots \\
=& X^{n-4}\left(X[P_x, X^3] - i\hbar X^3\right) - (n-3)i\hbar X^{n-1} \\
=& X^{n-3}\left(X[P_x, X^2]\right) - (n-2)i\hbar X^{n-1} \\
=& -nX^{n-1}.
\end{aligned} \tag{4.5}$$

Hence, due to the (4.5), (4.4) can be written as follows

$$[f(x), P_x] = i\hbar\left(\sum_{i=1}^{\infty} n a_n X^{n-1}\right) = i\hbar\frac{\partial f}{\partial x}. \tag{4.6}$$

which is equal to the formal definition. □

4.1.7 Exercise 4.7

For the region where $w = 0$

$$\left(\nabla^2 + k^2\right)\varphi(x) = 0; \quad \varphi(0) = \varphi(a) = 0; \quad \partial_x\varphi(0) = \partial_x\varphi(a) = 0 \tag{4.7}$$

where the first equation express the time-evolution with $k^2 = 2mE/\hbar^2$ (m is the particle's mass), and others two about boundary conditions. In this context, the general solution is

$$\varphi(x) = \lambda_1 \sin(kx) + \lambda_2 \cos(kx),$$

however, using the wave-function boundary condition we shall see that $\lambda_2 = 0$ and $k \to k_n := \frac{n\pi}{a}$. Symbolically,

$$\varphi_n(x) = \lambda_1 \sin\left(\frac{n\pi}{a}x\right). \quad n \in \mathbb{N} \tag{4.8}$$

Now, using the normalization (physical condition) $\varphi_n(x)$:

$$\int_0^a \mathrm{d}x\, |A|^2 \sin^2\left(\frac{n\pi}{a}x\right) = |A|^2\left(\frac{a}{2}\right) \implies A = \sqrt{\frac{2}{a}}.$$

Hence,

$$\varphi_n(x) = \sqrt{\tfrac{2}{a}} \sin\left(\frac{n\pi}{a}x\right). \tag{4.9}$$

Let be $\{\varphi_n(x)\}$. In terms of this basis, the operator X has the following matrix elements

$$X_{nm} = \frac{2}{a}\int_0^a \sin\left(\frac{n\pi}{a}x\right) x \sin\left(\frac{m\pi}{a}x\right). \tag{4.10}$$

Or

$$X \doteq \begin{bmatrix} a/2 & -\frac{32a}{9\pi^2} & 0 & -\frac{64a}{225\pi^2} & \cdots \\ -\frac{32a}{9\pi^2} & a/2 & -\frac{96a}{25\pi^2} & 0 & \cdots \\ 0 & -\frac{96a}{25\pi^2} & a/2 & -\frac{96a}{49\pi^2} & \cdots \\ -\frac{64a}{225\pi^2} & 0 & -\frac{96a}{49\pi^2} & a/2 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}.$$

In analogue for linear momentum operator, $P = i\hbar\partial_p$ (coordinates representation)

$$P_{nm} = -i\hbar\frac{2m\pi}{a^2}\int_0^a \sin\left(\frac{n\pi}{a}x\right)\cos\left(\frac{m\pi}{a}x\right)$$

or, in matrix form

$$P \doteq -\frac{i\hbar}{a}\begin{bmatrix} 0 & \frac{8}{3} & 0 & \frac{16}{15} & \cdots \\ -\frac{8}{3} & 0 & \frac{24}{5} & 0 & \cdots \\ 0 & -\frac{24}{5} & 0 & \frac{48}{7} & \cdots \\ -\frac{16}{15} & 0 & -\frac{48}{7} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}.$$

4.1.8 Exercise 4.8

In the regions $x < 0$ and $x > 0$ are, respectively,

$$\begin{aligned}(\nabla^2 + k_1^2)\psi_2 =& 0\\ (\nabla^2 + k_2^2)\psi_2 =& 0.\end{aligned}$$

With $k_1^2 := \frac{2m}{\hbar^2}(V_0+E)$, m is the electron mass, E their total energy and $k_2 := \frac{2mE}{\hbar^2}$. The solution of above equations (for $E > 0$) are equal to

$$\psi_1(x) = A_1\exp(ik_1x) + B_1\exp(-ik_1x) \qquad \psi_2(x) = A_2\exp(ik_2x) + \underbrace{B_2\exp(-ik_2x)}_{\text{vanish for a FP}}.$$

Firstly, let us make some remarks on the relationship between Energy-Transmission: initially if the energy spectrum are $-V_0 < E < 0$. Then, Let us assume (our hypothesis) that the electron can be ejected, hence, the total energy of the free electron are negative, which it is impossible once the Hamiltonian operator of a free particle is Hermitian (i.e. has positive eigenvalues). The same argument implies that E cannot be less than $-V_0$.

Fixing E as a positive number, and the 2-continuity ($\psi \in C_2$), we obtain:]

$$\begin{aligned}A_1 + B_1 &= A_2\\ ik_1(A_1 - B_1) &= ik_2A_2\end{aligned}$$

therefore

$$2k_1A_1 = (k_1 + k_2)A_2.$$

In this context, the transmission coefficient can be written as

$$T = \left|\frac{A_2}{A_1}\right|^2 \frac{k_2}{k_1} = \frac{4k_2/k_1}{(1+k_2/k_1)^2}$$

4.1.9 Exercise 4.9

The time-independent Schrödinger equation for $W(x) = C/r^2$. is

$$(\nabla^2 + k^2)\phi(\mathbf{x}) = \frac{2mC}{\hbar^2 r^2}\phi(\mathbf{x}),$$

with $k^2 := 2mE/\hbar^2$. Or, in spherical coordinates (e.g., $\nabla^2(\phi) = \frac{1}{r}\frac{\partial^2(r\phi)}{\partial r^2} + \nabla^2_{(\theta,\phi)}(\phi)$) in addition to the spherical symmetry of ϕ, we obtain:

$$\frac{1}{r}\frac{\partial^2}{\partial r^2}\left(rR(r)Y(\theta,\varphi)\right) + \nabla^2_{(\theta,\phi)}\left(R(r)Y(\theta,\varphi)\right) + k^2\left(R(r)Y(\theta,\varphi)\right) = \frac{2mC}{\hbar^2 r^2}\left(R(r)Y(\theta,\varphi)\right),$$

which implies that

$$\begin{cases} r\dfrac{\mathrm{d}^2}{\mathrm{d}r^2}(rR) + \left(r^2k^2 - \dfrac{2mc}{\hbar^2} - \lambda^2\right)R = 0; \\ \nabla^2_{(\theta,\phi)}Y + \lambda^2 Y = 0. \end{cases}$$

However again, via spherical symmetry of the problem, we must consider only the radial wave-function, moreover, in the asymptotic regime ($r \to 0$) we obtain:

$$r^2\frac{\mathrm{d}^2}{\mathrm{d}r^2}(rR) - \left(\frac{2mc}{\hbar^2} + \lambda^2\right)R = 0.$$

Now, we introduce the following auxiliary definition

$$\phi = u(r)/r.$$

Therefore, the radial differential equation assume the following form:

$$r^2\frac{\mathrm{d}^2u}{\mathrm{d}r^2} - \left(\frac{2mc}{\hbar^2} + \lambda^2\right)u = 0.$$

We can look for a solution as $u = r^s$, such that

$$r^s\left(s(s-1) - \left(\frac{2mc}{\hbar^2} + \lambda^2\right)\right) = 0.$$

Which the solution implies that

$$s_{\pm} = \frac{1 \pm \sqrt{1+\mu}}{2},$$

where $\mu = 4\left(\frac{2mc}{\hbar^2} + \lambda^2\right)$. However, note that, in the limit $r \to 0$ any negative power of r explode. In this scenario, the unique possibility of ϕ is

$$\phi(r) = Ar^{\mu_+ - 1}.$$

On the other hand, for this wave function has a physical significance the coefficient $\mu_+ - 1$ must be positive. Hence,

$$\frac{1+\sqrt{1+\mu}}{2} > 1 \implies C > \lambda^2.$$

It is not a propose here, but if we solve the angular part of this problem, we can obtain $\lambda^2 = -\hbar^2/2ml(l+1)$. Hence, $C > -\frac{\hbar^2}{2m}l(l+1)$ can describes a physical state.

4.1.10 Exercise 4.10

In the same way of the previously exercise, we have the following equation to the symmetric function $u(r)$

$$r^2\frac{\mathrm{d}^2u}{\mathrm{d}r^2} + \left[E - \frac{2mC}{\hbar^2}\frac{1}{r^n}\right]u = 0.$$

If $n \geqslant 2$ we can argue that any function r^l cannot describe a physical state. In the sense of, the potential W vanish rapidly than any r^l.

Therefore, one possibility is define $u(r)$ as an exponential

$$u(r) = \exp(-1/r^\gamma)f(r).$$

Like the preceding exercise, we shall determine condition to $u(r)$. In this scenario, we return the above equation into the differential equation one, the result of this evaluation is

$$\frac{a^2\gamma^2}{r^{2\gamma+2}} - \frac{C}{r^n} = 0.$$

Therefore, we must have $2\gamma + 2 = n$, and $a^2\gamma^2 = C$. Finally we get two physical condition: $1-$ the repulsive potential $a = C^{1/2}/\gamma$; $2-$ The attractive one, which occurs when a is a pure imaginary

4.1.11 Exercise 4.11

If $J = J(x)$ satisfied the continuity equation, then,

$$\partial_t|\psi|^2 + \nabla \cdot (J) = 0.$$

In this context, a new function $J \longrightarrow J' = J + f(x,t)$ only hold the continuity equation if and only if $\partial_x f(x,t) = 0$. Therefore, $f(x,t) = f(t)$. However, J has to be a limited function (i.e., $J(x,t)$ must be vanish in $x \to \infty$). The last condition implies that $f(x,t) \to 0$ in that limit, but this condition holds only if $f(x,t)$ is not a function of time. In the end, it is clear that J' only describes a physical probability flux when $f(x,t)$ is a null function.

4.1.12 Exercise 4.12

Due to the continuity of the wave function in addition to assumption $E > 0$:

$$\begin{pmatrix} 1 & 1 \\ ik_1 & -ik_1 \end{pmatrix} \begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ ik_2 & -ik_2 \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix}$$

$$\begin{pmatrix} \exp(ik_2 a) & \exp(-ik_2 a) \\ ik_2 \exp(ik_2 a) & -ik_2 \exp(-ik_2 a) \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix} = \begin{pmatrix} \exp(ik_1 a) & \exp(-ik_1 a) \\ ik_1 \exp(ik_1 a) & -ik_1 \exp(-ik_1 a) \end{pmatrix} \begin{pmatrix} A_2 \\ B_2 \end{pmatrix},$$

where $k_1^2 := 2mE/\hbar^2$ and $k_2^2 := 2m(V_0 + E)\hbar^2$.

The above pair equations can be solved in terms of a transfer matrix, P, where the element P_{11} is such that $T := \left|p_{11}^{-1}\right|^2$. In this scenario, we compute P_{11} via symbolic calculus in mathematica 12 (see the attached file). The results of that evaluation is written as

$$P_{11} = \exp(ik_1 a) \left[\cos(k_2 a) - \frac{i}{2} \left(\frac{k_1^2 + k_2^2}{k_1 k_2}\right) \sin(k_2 a)\right].$$

Hence, the transmission coefficient is computed via

$$\begin{aligned} T =& \left|p_{11}^{-1}\right|^2 \\ =& \left[\cos^2(k_2 a) + \frac{1}{4}\left(\frac{k_1^2 + k_2^2}{k_1 k_2}\right)^2 \sin^2(k_2 a)\right]^{-1} \end{aligned}$$

however,

$$\left(\frac{k_1^2+k_2^2}{k_1k_2}\right)^2 = \frac{V_0+4(V_0+E)E}{(V_0+E)E} = 1+\frac{V_0^2}{4(V_0+E)E}.$$

In other words, due to the constraint $R+T=1$:

$$T=\left[1+\frac{V_0^2}{4(V_0+E)E}\sin^2(k_2a)\right]^{-1},$$

and

$$R=\frac{V_0^2\sin^2(k_2a)}{4(V_0+E)E+V_0^2\sin^2(k_2a)}.$$

For $-V_0<E<0$ the exponential coefficients must be change as follows

$$\begin{pmatrix}1 & 1\\ \rho_1 & -\rho_1\end{pmatrix}\begin{pmatrix}A_1\\ B_1\end{pmatrix}=\begin{pmatrix}1 & 1\\ ik_2 & -ik_2\end{pmatrix}\begin{pmatrix}C\\ D\end{pmatrix}$$

$$\begin{pmatrix}\exp(ik_2a) & \exp(-ik_2a)\\ ik_2\exp(ik_2a) & -ik_2\exp(-ik_2a)\end{pmatrix}\begin{pmatrix}C\\ D\end{pmatrix}=\begin{pmatrix}\exp(\rho_1a) & \exp(-\rho_1a)\\ \rho_1\exp(\rho_1a) & -\rho_1\exp(-\rho_1a)\end{pmatrix}\begin{pmatrix}A_2\\ B_2\end{pmatrix},$$

where $ik_1\rightarrow\rho_1$. The P_{11} element is such that

$$P_{11}=\exp(\rho_1a)\left[\cos(k_2a)-\frac{i}{2}\left(\frac{V_0+2E}{\sqrt{E(V_0+E)}}\right)\sin(k_2a)\right].$$

With this new assignment, we can determine the transmission (same for reflection one) coefficient as

$$T=\exp(-2\rho_1a)\left[1+\frac{V_0^2}{4(V_0+E)E}\sin^2(k_2a)\right]^{-1},$$

and

$$R=\frac{V_0^2\sin^2(k_2a)}{4(V_0+E)E+V_0^2\sin^2(k_2a)}.$$

4.1.13 Exercise 4.13

This problem has the same principle that exercise 4.3, although we have two transfers matrix: $1-$ the first associated to the barrier $(0\rightarrow a)$ (which it is the same of the above exercise); $2-$ the second transfer matrix which represents the wave function flux through the last barrier $(b\rightarrow b+a)$

As we said, the first matrix was calculated in the exercise 4.3, therefore, we only have to evaluate the second and make their multiplication. Due to the continuity of the wave function and their derivatives, we have two conditions:

$$\begin{pmatrix} \exp(ikb) & \exp(-ikb) \\ ik\exp(ikb) & -ik\exp(-ikb) \end{pmatrix}\begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = \begin{pmatrix} \exp(\beta b) & \exp(-\beta b) \\ \beta\exp(\beta b) & -\beta\exp(-\beta b) \end{pmatrix}\begin{pmatrix} E \\ F \end{pmatrix}$$

$$\begin{pmatrix} \exp(\beta(b+a)) & \exp(-\beta(b+a)) \\ \beta\exp(\beta(b+a)) & -\beta\exp(-\beta(b+a)) \end{pmatrix}\begin{pmatrix} E \\ F \end{pmatrix} = M8\begin{pmatrix} A_3 \\ B_3 \end{pmatrix},$$

where $k^2 = 2mE/\hbar^2$, $\beta^2 = 2m/\hbar^2(V_0 - E)$, and

$$M8 = \begin{pmatrix} \exp(ik(b+a)) & \exp(-ik(b+a)) \\ ik\exp(ik(b+a)) & -ik\exp(-ik(b+a)) \end{pmatrix}.$$

With the Mathematica (see the code), we can solve the last pair of equation and obtain the second transfer matrix as

$$P_2 = \begin{pmatrix} e^{ika}\left[\cosh(\beta a) + \frac{i}{2}\left(\frac{\beta}{k} - \frac{k}{\beta}\right)\sinh(\beta a)\right] & \frac{i}{2k\beta}e^{-ik(a+2b)}(k^2+\beta^2)\sinh(\beta a) \\ -\frac{i}{2k\beta}e^{ik(a+2b)}(\beta^2+k^2)\sinh(\beta a) & e^{-ika}\left[\cosh(\beta a) - \frac{i}{2}\left(\frac{\beta}{k} - \frac{k}{\beta}\right)\sinh(\beta a)\right] \end{pmatrix}.$$

As T can be determined only with the element P^F_{11}, where the superscript F denotes the final matrix (i.e. product matrix be), we have

$$\begin{aligned} P^F_{11} =& \frac{1}{4k^2\beta^2}\big[e^{2ikb}(k^2+\beta^2)^2\sinh^2(\beta a) \\ &+ e^{2iak}(2k\beta\cosh(\beta a) - i(k^2-\beta^2)\sinh(\beta a))^2\big]. \end{aligned}$$

With this coefficient we can obtain T, via $T = \left|1/P^F_{11}\right|^2$, however, the computation of this quantity is a hard task... then we leave for the enthusiastic reader!

4.1.14 Exercise 4.14

In the coordinates representation (one-dimensional), the Schrödinger's time-independent equation (SE) for a delta potential assumes the following forms

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + C\delta(x)\psi = -k^2\psi,$$

where $C = -2m/\hbar^2 a$ ($a \in \mathbb{R}$), and $k^2 = 2mE/\hbar^2$. Now, integrating the above equation in a finite interval, we obtain

$$\begin{aligned}\int_{-\epsilon}^{\epsilon} \mathrm{d}x \, \frac{\mathrm{d}}{\mathrm{d}x} \frac{\mathrm{d}\psi}{\mathrm{d}x} + C \int_{-\epsilon}^{\epsilon} \mathrm{d}x \, \delta(x)\psi =& \frac{\mathrm{d}\psi}{\mathrm{d}x}(\epsilon) - \frac{\mathrm{d}\psi}{\mathrm{d}x}(-\epsilon) + C\psi(0) \\ =& - k^2 \left[F[\psi](\epsilon) - F[\psi](-\epsilon)\right].\end{aligned}$$

With $F[\psi]$ being the primitive function of ψ. However, the wave equation must be a continuous function, in this sense, $F[\psi]$ is a continuous function. With the last assumption in our minds, we compute the limit when ϵ goes to zero:

$$\frac{\mathrm{d}\psi_+}{\mathrm{d}x}(0) - \frac{\mathrm{d}\psi_-}{\mathrm{d}x}(0) + C\psi(0) = 0.$$

Note that the above equation proves that, due to the delta potential, the first derivative of $\psi(x)$ has a discontinuity. In other words, in this case, a truly physical wave function must to satisfy the SE and the discontinuity (above formula).

For item B: we have to ensure that $E < 0$, otherwise, the "particle" cannot be a ground state (except to the trivial one). For negative $ik \to \rho$, then the solutions of SE are

$$\psi_\pm(x) = A_\pm \exp(\rho x) + B_\pm \exp(-\rho x).$$

Nevertheless, this solutions also have to satisfy the discontinuity rule, and more, they have to vanish in $|x| \to \infty$. The last condition tell to us that $A_+ = B_- = 0$, on other hand, for the discontinuity

$$\psi'_+(0) - \psi'_-(0) = - \rho(B_+ + A_-) = -2mc/\hbar^2 \psi(0),$$

where we used that $W(X) = -c\delta$ ($c \in \mathbb{R}$). However, $\psi(x)$ is a continuous function, hence,

$$A_- = B_+ \equiv D \implies \psi(0) = D.$$

Therefore, the two above equations given the following identities: First,

$$\psi(0) = D;$$

and finally

$$\rho = \frac{mc}{\hbar^2} = \sqrt{-\frac{2mE}{\hbar^2}} \implies E = -\frac{mc^2}{\hbar^2}.$$

Note that energy level is unique and therefore represents a ground state for this potential.

Return to the wave equation, let us define the normalization constant D:

$$\int_{-\infty}^{+\infty} \mathrm{d}x \, |\psi(x)|^2 = |D|^2 \left[\int_{-\infty}^{0} \mathrm{d}x \exp(2\rho x) + \int_{0}^{\infty} \mathrm{d}x \exp(-2\rho x) \right] = |D|^2/\rho = 1.$$

Hence,

$$\psi(x) = \sqrt{\frac{mc}{\hbar^2}} \exp\Big(-\frac{mc}{\hbar^2}|x|\Big).$$

4.1.15 Exercise 4.15

The Lagrangian of a free particle in the path $(x_1, t_1) \to (x_2, t_2)$ is

$$\begin{aligned} L =& \frac{m}{2}\dot{x}^2 \\ =& \frac{m}{2}\left(\frac{x_2 - x_1}{t_2 - t_1}\right)^2. \end{aligned}$$

in this scenario, the action is determined as

$$S = \int_{t_1}^{t_2} L \, \mathrm{d}t = \frac{m}{2} \frac{(x_2 - x_1)^2}{t_2 - t_1}.$$

Hence, the Fyemann phase factor is

$$\exp(iS/\hbar) = \exp\big(i \tfrac{mv}{2\hbar}(x_2 - x_1)\big) = \exp(i\pi(x_2 - x_1)\lambda).$$

where λ is the de Broglie wavelength, and $v = (x_2 - x_1)/(t_2 - t_1)$.

4.1.16 Exercise 4.16

Consider the Schrödinger non-homogeneous equation as follows

$$\left(H_x - i\hbar\frac{\partial}{\partial t}\right)\Psi(x;t) = F(x;t),$$

where, H_x is the Hamiltonian in x-representation. Then, a Green function correspondent to this problems satisfy:

$$\left(H_x - i\hbar\frac{\partial}{\partial t}\right)G(x,t;x',t_0) = -i\hbar\delta(t - t_0)\delta(x - x'),$$

Now, we can prove that $G(x,t;x',t_0) = \big\langle x \big| U(t,t_0) \big| x' \big\rangle$ satisfies the above condition.

Proof. For a forward time evolution, the unitary operator of time evolution can be written as

$$U(t,t_0) \coloneqq \exp(-iH(t-t_0)/\hbar).$$

By a directly evaluation, we obtain

$$\begin{aligned} i\hbar\partial_t(\Theta(t-t_0)\left\langle x\middle|U(t,t_0)\middle|x'\right\rangle) =& i\hbar\frac{\mathrm{d}\Theta}{\mathrm{d}t}(t-t_0)\left\langle x\middle|U(t,t_0)\middle|x'\right\rangle \\ &+ \Theta(t-t_0)\left\langle x\middle|i\hbar\partial_t U(t,t_0)\middle|x'\right\rangle \\ =& i\hbar\delta(t-t_0)U(t,t_0) \\ &+ \Theta(t-t_0)\left\langle x\middle|HU(t-t_0)\middle|x'\right\rangle. \end{aligned}$$

However, note that Θ is a multiple of the identity and U is a function of H, hence, both operator commute with the Hamiltonian. Moreover, H_x is such that

$$H_x\psi(x) = \langle x|H|\psi\rangle.$$

Then let be $|\psi\rangle \coloneqq \Theta(t-t_0)U(t,t_0)$ in the last pair of equations:

$$\begin{aligned} i\hbar\partial_t(\Theta(t-t_0)\left\langle x\middle|U(t,t_0)\middle|x'\right\rangle) =& i\hbar\delta(t-t_0)\left\langle x\middle|U(t,t_0)\middle|x'\right\rangle \\ &+ \left\langle x\middle|H\left(\Theta(t-t_0)U(t-t_0)\right)\middle|x'\right\rangle. \end{aligned}$$

As for the first term on the right-hand side, the δ vanishes for any $t \neq t_0$, so we can use that $U(t_0,t_0) = \mathbb{1}$ for obtain:

$$(H_x - i\hbar\partial_t)\left(\Theta(t-t_0)\left\langle x\middle|U(t,t_0)\middle|x'\right\rangle\right) = -i\hbar\delta(t-t_0)\delta(x-x_0).$$

Now, we must solve the Green function to $H = P^2/2m$. In this scenario the SE for G as

$$\left(\frac{\partial}{\partial t} - a^2\frac{\partial^2}{\partial x^2}\right)G = \delta(t-t_0)\delta(x-x_0).$$

With was set $a^2 = \frac{i\hbar}{2m}$. Taking the Fourier transform in relation to G (i.e.,$G_F = \mathcal{F}(G)$) of this equation we obtain

$$\frac{\partial G_F}{\partial t} + x_0^2a^2\frac{\partial^2 G_F}{\partial x^2} = \frac{\exp(ikx_0)}{\sqrt{2\pi}}\delta(t-t_0).$$

A nice trick in the last equation is take down their Laplace transformation. By definition, the Laplace transformation is

$$\mathcal{L}\{f(t)\} = \int_0^\infty \mathrm{d}\tau\, e^{-s\tau} f(\tau),$$

moreover, it is useful introduce the Laplace's transformation of $f'(t)$:

$$\mathcal{L}\{f'(t)\} = \mathcal{L}\{f(t)\} - f(0).$$

As our problem has an initial condition given by $G(0) = 0$, the Laplace transformation is simple. The computation of this is an algebraic equation to $\mathcal{L}(G) = G_{SF}$

$$sG_{SF} + x_0^2 a^2 G_{SF} = \frac{\exp(ikx_0)}{\sqrt{2\pi}} e^{-st_0}.$$

or, via $\mathcal{L}^{-1}\{\exp(-sa)/(s+a)\} = \mathcal{L}^{-1} 1/(s+a)\Theta(t-a)$ we can rearrange as

$$G_F = \frac{\exp(ikx_0)}{\sqrt{2\pi}} \exp\bigl(-a^2k^2(t-t_0)\bigr)\Theta(t-t_0),$$

or, in terms of x coordinates

$$\begin{aligned} G =& \Theta(t-t_0)\frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}k \exp(-ikx)\exp(ikx_0)\exp\bigl(-a^2k^2(t-t_0)\bigr) \\ =& \Theta(t-t_0)\frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}k \exp(-ik(x-x_0))\exp\bigl(-a^2k^2(t-t_0)\bigr). \end{aligned}$$

Moreover, the above solution has a general solution as follows

$$\int_{-\infty}^{\infty} \mathrm{d}u \exp\bigl(-a^2u^2\bigr)\exp(bu) = \sqrt{\pi/a}\exp\bigl(b^2/4a\bigr).$$

Therefore, in our context

$$G(x,t;x_0,t_0) = \Theta(t-t_0)\left(\frac{m}{4\pi i\hbar(t-t_0)}\right)^{1/2} \exp\left(\frac{im(x-x_0)^2}{2\hbar(t-t_0)}\right).$$

□

4.1.17 Exercise 4.17

The propagator is the solution of

$$G(x,t;x_0,t_0) = \int \mathcal{D}(x)\exp(iS/\hbar),$$

where $\mathcal{D}(x)$ is a measure based in every possible trajectories between $(x_0, t_0) \to (x, t)$, and S is the action of the system. However, if we assume only the classical path to the free particle, we obtain

$$G = \exp\left(i\frac{m}{2\hbar}\frac{(x-x_0)^2}{t-t_0}\right)\int_{cp} \mathrm{d}x(\tau)\,.$$

With the last integral being a kind of sum over all possible classical paths of the particle. Assuming that $x(\tau) = x(\tau) + \delta x(\tau)$ (classical), in the limit of large paths $N \to \infty$, we conclude that

$$\int_{cp} \mathrm{d}x(\tau) \to \left(\frac{m}{4\pi i\hbar(t-t_0)}\right)^{1/2}.$$

Hence,

$$G(x,t;x_0,t_0) = \left(\frac{m}{4\pi i\hbar(t-t_0)}\right)^{1/2}\exp\left(\frac{im(x-x_0)^2}{2\hbar(t-t_0)}\right).$$

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