Simulation of Quantum Computing Models

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Purpose:

This paper was done to familiarize myself with some of the basic concepts of Quantum Computing. It was a learning experience for me. This work provides **Quantitative Solutions and Simulations** for Quantum Computing (QC) models and examples. This material has been gathered from a number of QC books and papers. A list of some the books and papers used in this analysis are given at the end of this work. This is not original work. It is a compendium of various books and research papers.The goal is to capture basic Quantum Computing Concepts and Models using the mathematical tools provided by Mathcad and Mathematica. We use this methodology to Simulate various Quantum Mechanical and Quantum Computing Phenomena.

Mathcad operations are shown in purple italics.

For example: $sin\left(\frac{\pi}{2}\right) = 1$

Perspective:

When I took courses in Quantum Mechanics (QM) many years ago, the concepts and operations involved in QM seemed very foreign and abstract. The availability of Programming Languages that can capture the mathematics symbolically, has now made it possible to easily do mathematical operations and explore QM models, simulations, solutions, and plots of abstract math. The capability for these manipulations was unimaginable when I first studied QM. Being able to reproduce the original numerical results, and in particular, being able to run simulations and make the results visible with 2-D and 3-D graphics, which can be tilted, rotated, contrasted, thus being able to examine geometric details in phase space, has in some sense, mastered and made explicit many of the complexities of this subject. This work has been great fun.

This Mathcad File is available at: VXPhysics.com/Mathcad

Mathcad Simulation Methodology

Simulation of quantum computers generally involves representing quantum states and operators in linear algebra and applying transformations in accordance with quantum mechanics. This is usually done in languages like Python, which have libraries like Qiskit, Cirq, and Pennylane specifically built for quantum computing.

However, theoretically, it is possible to simulate simple quantum systems using Mathcad because at its core, quantum mechanics relies heavily on Linear Algebra, Matrix Mechanics, Vector Tensor Products, and solutions of Eigenvalue Equations, all of which Mathcad can easily accommodate. For example, we will represent qubits (quantum bits) as vectors and quantum gates as matrices and perform matrix multiplication to simulate the application of quantum gates to qubits. The | and > symbols needed to define the names for the states of Dirac Notation, e.g. |Ψ> are only available as text in Mathcad. The results of these operations can be calculated using Mathcad operators and functions, but the Dirac Notation symbols cannot be used as as the Names for the associated variables or functions.

Summary

The past few decades have witnessed a paradigm shift in computational sciences with the advent of quantum computing, a cutting-edge technology promising to revolutionize data processing by leveraging quantum mechanical phenomena. This paper delves into the intricate concepts that underpin quantum computing and their simulation, providing an extensive exploration of this domain that ranges from its fundamental principles to intricate quantum algorithms.

Beginning with a historical overview, we journey through the genesis and development of quantum computing, setting a solid foundation upon which to build a comprehensive understanding of the field. We delve into the six postulates of quantum mechanics and Dirac's relativistic matrix mechanics, pivotal in understanding the theoretical framework of quantum physics. To clarify these complex theories, we illuminate the mathematical formulations of quantum mechanics through Dirac notation, vector, matrix, and Tensor Product mathematics.

We then explore the enigmatic phenomena at the heart of quantum mechanics: superposition, entanglement, and quantum operators. By investigating experiments such as the 3 Polarizer Paradox and Stern-Gerlach, we seek to bring clarity to these seemingly paradoxical phenomena.

The exploration of quantum mechanics would be incomplete without a dive into its most transformative applications: quantum algorithms. The paper discusses fundamental quantum algorithms like Deutsch, Deutsch-Jozsa, Shor's factoring algorithm, and Grover's search algorithm. These algorithms, running on quantum computers, have the potential to solve problems significantly faster than classical computers, thus underscoring the power of quantum computing.

In addition, we simulate key principles and operations in quantum mechanics, like the Aharonov-Bohm effect and the solution of the Schrödinger wave equation for the propagation of an electron. By probing the quantum eraser and the unique characteristics distinguishing fermions from bosons, we strive to illuminate the idiosyncrasies of the quantum world.

Throughout this exploration, our objective is not merely to understand quantum computing, but to demystify it, to bring it into the realm of the comprehensible, and to simulate these phenomena using classical analytic math tools such as Mathcad or Mathematica.

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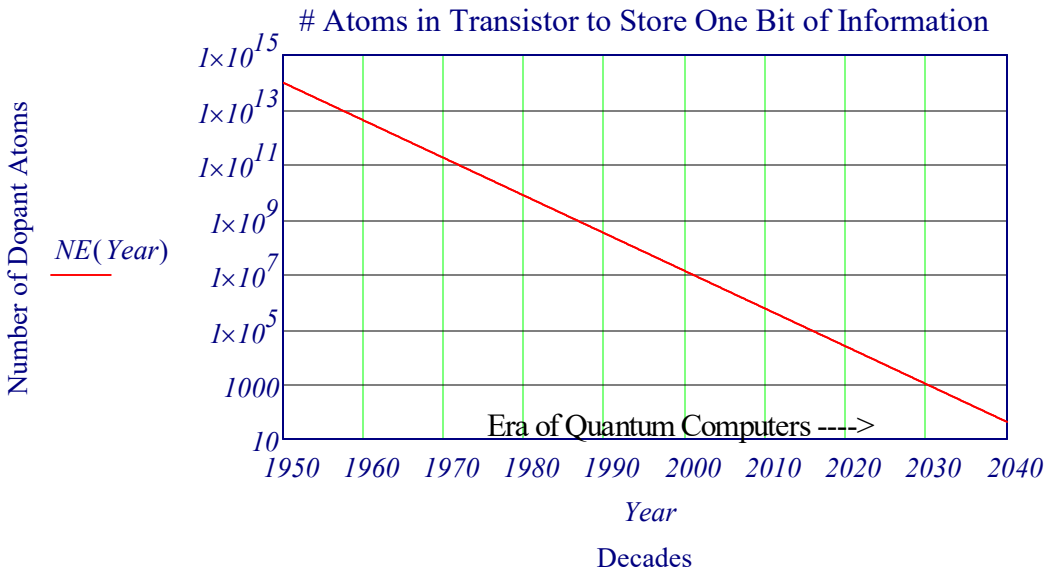
I. Introduction

With the development of science and technology, leading to the advancement of civilization, new ways were discovered exploiting various physical resources such as materials, forces and energies. The history of computer development represents the culmination of years of technological advancements beginning with the early ideas of Charles Babbage and eventual creation of the first computer by German engineer Konard Zeise in 1941.

The number of atoms needed to represent a bit of memory has been decreasing exponentially since 1950. An observation by Gordon Moore in 1965 laid the foundations for what came to be known as "Moore's Law" – that computer processing power doubles every eighteen months. If Moore's Law is extrapolated naively to the future, it is learnt that sooner or later, each bit of information should be encoded by a physical system of subatomic size. The plot below shows the number of electrons required to store a single bit of information. An extrapolation of the plot suggests that we might be within the reach of atomic scale computations with in a decade or so at the atomic scale however. This is the point at which Moore's Law for a transistor (not the architecture of the integrated circuit system) and the **exponential growth** of classical computers comes to an end.

Decrease in the Number of Electrons Needed Per Bit Versus Years (TWK Estimate)

$$NE(Y) := 10^{\left(14-11\cdot\frac{Y-1950}{80}\right)}$$



Dimensions of 3 nm Node Transistor: 4nm x 42 nm x 5nm

Volume of Transistor, V_{xtr}

$$V_{xtr} := 4nm\cdot 42nm\cdot 5nm$$

Density of Silicon atoms per m^3:

$$\rho_{Si} := 5\cdot 10^{28}\cdot\frac{1}{m^3}$$

$$NumAtoms := V_{xtr}\cdot\rho_{Si}$$

$$NumAtoms = 42000$$

How does Quantum Computing Work? An interview with Peter Shor, discoverer of the *Shor Algorithm*.

Peter Shor: "The key to factoring is identifying prime numbers, which are whole numbers divisible only by one and by themselves. (Five is prime. Six, which is divisible by two and by three, is not.) There are twenty-five prime numbers between one and a hundred, but as you count higher they become increasingly rare." Shor, drawing a series of compact formulas on the chalkboard, explained that certain sequences of numbers repeat periodically along the number line. The distances between these repetitions grow exponentially, however, making them difficult to calculate with a conventional computer.

"O.K., here is the heart of my discovery," he said. "Do you know what a diffraction grating is?" I confessed that I did not, and Shor's eyes grew wide with concern. He began drawing a simple sketch of a light beam hitting a filter and then diffracting into the colors of the rainbow, which he illustrated with colored chalk. "Each color of light has a wavelength," Shor said. "We're doing something similar. This thing is really a computational diffraction grating, so we're sorting out the different periods." Each color on the chalkboard represented a different grouping of numbers. A classical computer, looking at these groupings, would have to analyze them one at a time. *A quantum computer could process the whole rainbow at once*."

What is a Quantum Computer (QC)?

Qubit: A qubit is a **two-dimensional system** that is in a state of 0 or 1 or both. Just as a classical bit has a state – either 0 or 1, a qubit also has a state. Two possible states for a qubit are the states |0> and |1> , which as you might guess correspond to the states 0 and 1 for a classical bit. Notation like ' |> ' is called the *Dirac notation.*
Quantum Computing: A type of computation whose operations can harness the phenomena of quantum mechanics, such as superposition, interference, entanglement, and teleportation. Devices that perform quantum computations are known as quantum computers. Operations are done by gates. **All Operators in QC are reversible.**

The qubit is represented by the superposition of the two spin basis vectors in Hilbert space given by: A linear combination of the two gives what is called the single qubit state
$|\Psi = \alpha\,|1\rangle + \beta\,|0\rangle$, where α and β are the probability amplitudes and give the probability that an observation of the spin will result in |1> or a |0> state respectively

$$|1\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$|0\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

We can model a qubit computationally:

$|\varphi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle$ where $|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ where $\alpha^2 + \beta^2 = 1$, α and β are complex numbers.

If a qubit gets measured, it will return a classical bit value of 0 with probability of α^2 or a bit value of 1 with probability β^2.

Potential Applications: Cyber Security, Factorization, Breaking Codes (RSA), Simulate Quantum Phenomena. Rapid Prototyping and Testing of Chemical Reactions, Electronic and Material Properties, Molecular Folding, Calculating Fourier Transforms, Finding Solutions to a system of nonlinear equations, e.g. the Quantum Navier-Stokes Algorithm.

QC Key Concepts: Quantum Behavior, Superposition, Entanglement, Interference, Teleportation, "Oracle" Algorithms, Computational Complexity/Scaling, Born Rule, Reversibility, and of the Physics of states in a quantum system.

Computational Complexity: Computational complexity studies the amount of time and space required to solve a computational problem. Another measure is the number of gates & depth of circuit. Another important computational resource is energy. Energy consumption in computation turns out to be deeply linked to the reversibility of computation.

Reversibility: Consider a gate like the NAND gate, which takes as input two bits, and produces a single bit as output. This gate is intrinsically *irreversible* because, **given the output of the gate, the input is not uniquely determined**. The gate is an example of a reversible logic gate because, given the output of the gate, it is possible to infer what the input must have been. NAND Gate: A Boolean operator which gives the value zero if and only if all the operands have a value of one, and otherwise has a value of one (equivalent to NOT AND).

Erasure: Another way of understanding irreversibility is to think of it in terms of information erasure. If a logic gate is irreversible, then some of the information input to the gate is lost irretrievably when the gate operates – that is, some of the information has been erased by the gate. A computation is reversible if no information is erased during computation. Landauer's principle states that, in order to erase information, it is necessary to dissipate energy. A minimum of kBT ln2.

Entanglement is a different way of encoding information. If we have two particles that are entangled, the information about them is **not encoded locally in each particle**, but rather in correlation of the two. This is the Principle of Non Locality.

Algorithms: Shor's (Factorization), Deutsch–Jozsa., Grover's (Search), Bernstein–Vazirani, Quantum phase estimation.

Measurements: Every measurable physical quantity, o, is described by a corresponding Hermitian operator, O, acting on the state ψ. The eigenvalues of Hermetian operators are always real. Example: $H_{op}\psi = E\psi$ gives the Eigenvalue of Energy for state ψ. For every classically defined Function $F(x,p) \exists F_{op} = F(x, h/i\ d/dx$

The Poisson Bracket Formulation for the momentum operator: $\dot{p}_k = \{p_k, H\}$

Obstacles: Decoherence, Error Correction, Scalability (need to scale to 1000 Bits for "practical" applications). "Operating a quantum computer is a race against the clock." The same phenomenon enabling the potential computing power of quantum computers — entanglement — is also responsible for decoherence when it occurs with unmonitored degrees of freedom. The main challenge of quantum computing is to quickly build entanglement between the qubits before imperfections or decoherence overly corrupt the quantum state. This decoherence is an intrinsic characteristic of any quantum computer and its origin and consequences must be understood thoughtfully. But in all hardware realizations, it means each operation incurs a loss of fidelity relative to the ideal target quantum state."
What Limits the Simulation of Quantum Computers? Yiqing Zhou, PHYSICAL REVIEW X 10, 041038 (2020)

II. A Brief History of Quantum Computing

In 1961, Rolf Landauer stated the following Principle: An irreversible change in information stored in a computer, such as merging two computational paths, dissipates a minimum amount of heat (per bit) to its surroundings, $E \geq k_b * T * \ln 2$, where k_b is Boltzmann's constant. This principle asserts that all information is physical. This Law established a fundamental energy limits on computation. This limit can be transcended in QC by using reversible computing gates. Some people refer to Landauer as the "Godfather of quantum computation."

In 1981, Richard Feynman gave a lecture entitled "Simulating Physics with Computers" In this talk, he argued that a classical system could not simulate quantum phys cis. At the quantum level, all Physics is time reversible, but classical Physics, because of entropy, is not.

In 1985, David Deutsch, a physicist at Oxford, suggested a more comprehensive framework for quantum computing in his 1985 paper. In this work, he describes in detail what a quantum algorithm would look like.
He gave an algorithm that would **run exponentially faster** than **any possible deterministic classical** algorithm.

In 1993, Umesh Vazirani and his student Ethan Bernstein (BV) picked up where Deutsch and Jozsa left off. described an algorithm that showed clear quantum-classical separation even when small errors are allowed.

In 1994, Shor was a researcher in the mathematical division of Bell Labs in New Jersey. Shor studied the work of Deutsch, BV and Simon and realized he could construct an algorithm for factoring large numbers into two prime factors; factoring large numbers is believed to be intractable on a classical computer.

In 1999-2001, Yasunobu Nakamura built and demonstrated a functioning, controllable superconducting qubit. Nakamura used Josephson junctions to create a two-level system.

In 1995, Cirac and Zoller proposed an ion trap as the physical system to perform quantum computation.
In 1995, Grover developed the fastest possible quantum algorithm (O(N1/2)) for searching an unsorted database.

1996 Shor and Robert Calderbank, and independently Andrew Steane, saw a way to finesse the seemingly show-stopping problems of quantum mechanics to develop quantum error correction techniques. Today, quantum error correction is arguably the most mature area of quantum information processing.

2023 IBM Unveils 433 Qubit-Plus Quantum Processor. IBM expects to offer a 10000 qubit machine in 2025. Its qubits known as **transmons**, which are essentially **superconducting resonators** that can **store 0 or 1 microwave photons.** These qubits can be manipulated by applying microwave pulses of different frequencies to them from outside the processor, connected to each other with busses, different frequencies, can control them independently, passive microwave circuitry, which does not deliberately absorb or emit microwave signals but redirects them, microwave resonators that measure the state of the qubits, filters that protect the qubits from decaying out of a drive line, and transmission lines that deliver microwave signals to the qubits and to and from the readouts. Temp = 0.02K

III. Six Key Postulates of Quantum Mechanics

Physical Chemistry, Engel, Read, 3rd Ed 2014

Quantum mechanics can be formulated in terms of six postulates. Postulates cannot be proven, but they can be tested. The five postulates discussed in this chapter provide a framework for summarizing the basic concepts of QM.

POSTULATE 1

The state of a quantum mechanical particle is **completely specified by a wave function.**The state of a physical system is represented by a normalized ket in a Hilbert space ***H***. To simplify the notation, only one spatial coordinate is considered. The probability that the particle will be found at time t_0 in a spatial interval of width centered at x_0 is given by

$$P(x_0, t_0) = \Psi^*(x_0, t_0)\Psi(x_0, t_0)\, dx = |\Psi(x_0, t_0)|^2\, dx$$

The wave function must be a single-valued function of the spatial coordinates. If this were not the case, a particle would have more than one probability of being found in the same interval.

POSTULATE 2

For every measurable property of a system such as position, momentum, and energy, **there exists a corresponding operator in quantum mechanics**. An experiment in the laboratory to measure a value for such an observable is simulated in the theory by operating on the wave function of the system with the corresponding operator. All quantum mechanical operators belong to a mathematical class called Hermitian operators that have real eigenvalues. For a Hermitian operator $\hat{A}$, $\int \psi^*(x)[\hat{A}\psi(x)]\, dx = \int \psi(x)\,[\hat{A}\ \psi\ (x)]^* dx$

POSTULATE 3 (Born's Rule)

In any single measurement of the observable that corresponds to the operator, the **only** values that will ever be measured are the **eigenvalues** of that operator $\hat{A}$

POSTULATE 4

If the system is in a state described by the wave function, and the value of the observable a is measured once on each of many identically prepared systems, the average value (also called the expectation value) of all of these measurements is given by the normalized wavefunction

$$\langle a \rangle = \int \Psi^*(x,t)\hat{A}\Psi(x,t)dx$$

As we know, two cases apply with regard to *Ψ(x,t)*: it either is or is not an eigenfunction of the operator ^A. These two cases need to be examined separately. The state space of a composite physical system is the **tensor product** (**See Section VI**) of the state spaces of the component physical systems. If we have systems number 1 to n, prepared in state $|\psi_i\rangle$, then the joint state is of the total system is: $|\psi_1\rangle \otimes |\psi_2\rangle \otimes \cdots \otimes |\psi_n\rangle$

POSTULATE 5

The evolution in time of a quantum mechanical system is governed by the time-dependent Schrödinger equation:

$$\hat{H}\ \Psi(x,t) = i\hbar\frac{\partial\Psi(x,t)}{\partial t}$$

POSTULATE 6 (See **Section V**)

Quantum superposition is a fundamental principle of quantum mechanics. In classical mechanics, things like position or momentum are always well-defined. We may not know what they are at any given time, but that is an issue of our understanding and not the physical system. In quantum mechanics, a particle can be **in a superposition of different states**. It can be in **two places at once** (see double-slit experiment). A measurement always finds it in one state, but before and after the measurement, it interacts in ways that **can only be explained by having a superposition of different states.** A simple demonstration of superposition can be made using a beam of light that passes through a polarizing filter.

IV. Dirac's Relativistic Matrix Mechanics

Introduction to Quantum Mechanics, C. W Sherwin, *Physical_and_Theoretical_Chemistry,* Frank Rioux

In 1928, P.A.M. Dirac derived a **relativistic formulation of the quantum mechanics of fermions**. The equation is invariant under a Lorentz transformation and spin emerges as a natural consequence of the relativistic treatment.

The Relativistic Equation for the energy of a free particle has positive and negative roots, where the positive root signifies the energy of a particle and the negative root the energy of its antiparticle. This interpretation was confirmed experimentally with the discovery of the anti-electron (positron) in 1932 by Anderson.

$$E = \pm c\sqrt{p_x^2 + p_y^2 + p_z^2 + m^2c^2} \qquad (1)$$

Dirac converted this to a soluble quantum mechanical operator by first writing the argument of the square root as a perfect square in order to get rid of the troubling radical operator which defied physical interpretation. In a second step he replaced energy and momentum with their differential operators, $E = -(h/2\pi i)d/dt$ and $p_q = (h/2\pi i)d/dq$, from non-relativistic quantum mechanics. **Math**

$$p_x^{\,2} + p_y^{\,2} + p_z^{\,2} + m^2 \cdot c^2 = \left(\alpha_x \cdot p_x + \alpha_y \cdot p_y + \alpha_z \cdot p_z + \beta \cdot m \cdot c\right)^2$$

For this mathematical maneuver **to be valid** the following conditions must hold: $\alpha_x^{\,2} = \alpha_y^{\,2} = \alpha_z^{\,2} = \beta^2 = 1$

$$\alpha_x \cdot \alpha_y + \alpha_y \cdot \alpha_x = 0 \qquad \alpha_x \cdot \alpha_z + \alpha_z \cdot \alpha_x = 0 \qquad \alpha_x \cdot \beta + \beta \cdot \alpha_x = 0 \qquad \alpha_y \cdot \alpha_z + \alpha_z \cdot \alpha_y = 0$$

$$\alpha_y \cdot \beta + \beta \cdot \alpha_y = 0 \qquad \alpha_z \cdot \beta + \beta \cdot \alpha_z = 0 \qquad p_x \cdot p_y = p_y \cdot p_x \qquad p_x \cdot p_z = p_z \cdot p_x \qquad p_y \cdot p_z = p_z \cdot p_y$$

In other words, the **αs and βs must anticommute** while the momentum operators as used above **must commute**. From the non-relativistic formulation of quantum mechanics it was already clear that the momentum operator pairs above did commute. In formulating a relativistic quantum mechanics, Dirac assumed the validity of the various multiplicative and differential operators of non-relativistic quantum mechanics for observable properties like energy, position and momentum.

Being aware of **Heisenberg's matrix approach** to non-relativistic quantum mechanics, Dirac realized the restrictions above regarding the as and b could be satisfied by the following 4x4 matrices. These matrices are formed from the **Pauli X, Y, Z Basis Matrices ($\sigma_x, \sigma_y, \sigma_z$) are** Unitary Hermetian Matrices. Hermitian operators represent observables in quantum mechanics, so the Pauli matrices span the space of observables of the complex 2 dimensional Hilbert space. **See Section VIII**. Stern-Gerlach Experiment for more on the Pauli Spin Matrices.

Mathcad Matrix Formulation

$$\sigma_x := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_z := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\sigma_1 := \sigma_x \qquad \sigma_2 := \sigma_y \qquad \sigma_3 := \sigma_z$$

I is the Identity operator. $I := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$

$$\alpha_x := \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \quad \alpha_y := \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix} \quad \alpha_z := \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix} \quad \beta := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

First we show that $\alpha_x^2 = \alpha_y^2 = \alpha_z^2 = \beta^2 = 1$

$$\alpha_x \cdot \alpha_x = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad \alpha_y \cdot \alpha_y = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad \alpha_z \cdot \alpha_z = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad \beta \cdot \beta = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Now we show that the **αs and β s anticommute:** $\sigma_i\sigma_j + \sigma_j\sigma_i = 0$ **Noncommutability of measurements in QM.**

$$\alpha_x \cdot \alpha_y + \alpha_y \cdot \alpha_x = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad \alpha_x \cdot \alpha_z + \alpha_z \cdot \alpha_x = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad \alpha_x \cdot \beta + \beta \cdot \alpha_x = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$\alpha_y \cdot \alpha_z + \alpha_z \cdot \alpha_y = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad \alpha_y \cdot \beta + \beta \cdot \alpha_y = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad \alpha_z \cdot \beta + \beta \cdot \alpha_z = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

It is now possible to write Dirac's relativistic energy equation as follows:

$$\sigma_x \cdot \sigma_y + \sigma_y \cdot \sigma_x = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$$

$$E = \pm c\left(\alpha_x p_x + \alpha_y p_y + \alpha_z p_z + \beta mc\right) \qquad (2)$$

Before proceeding to the next step, the **substitution of the differential operators** for energy and momentum, it is instructive to look at the right side of the above equation which is a **4x4 Dirac relativistic energy operator**. Of course, the left side is a 4x4 matrix with **Energy, E, on the diagonal** and zeros everywhere else.

Note: *The **arrow symbol** → below is used in Mathcad to evaluate an expression symbolically. Mathcad returns the result as another expression in terms of the variable and symbols in the original problem.*

$$-c\cdot\left(\alpha_x\cdot p_x + \alpha_y\cdot p_y + \alpha_z\cdot p_z + \beta\cdot m\cdot c\right) \rightarrow \begin{bmatrix} -c^2\cdot m & 0 & -c\cdot p_z & -c\cdot\left(p_x - p_y\cdot i\right) \\ 0 & -c^2\cdot m & -c\cdot\left(p_x + p_y\cdot i\right) & c\cdot p_z \\ -c\cdot p_z & -c\cdot\left(p_x - p_y\cdot i\right) & c^2\cdot m & 0 \\ -c\cdot\left(p_x + p_y\cdot i\right) & c\cdot p_z & 0 & c^2\cdot m \end{bmatrix}$$

Substituting the traditional operators for energy and momentum yields,

$$-\frac{\hbar}{i}\frac{\partial \Psi}{\partial t} = -\left[\frac{c\hbar}{i}\left(\alpha_x \frac{\partial}{\partial x} + \alpha_y \frac{\partial}{\partial y} + \alpha_z \frac{\partial}{\partial z}\right) + \beta mc^2\right]\Psi \qquad (4)$$

Assuming the separability of the space and time coordinates [$\Psi(x,y,z,t) = \psi(x,y,z)\phi(t)$], **this four dimensional** differential equation is decoupled in to two differential equations. The time-dependent equation is easily solved and has the following solution.

$$\varphi(t) = e^{-i\frac{Et}{\hbar}} \qquad (5)$$

The space part of the differential equation has the following form, with the relativistic Hamiltonian operating on the wave function.

$$-\left[\frac{c\hbar}{i}\left(\alpha_x \frac{\partial}{\partial x} + \alpha_y \frac{\partial}{\partial y} + \alpha_z \frac{\partial}{\partial z}\right) + \beta mc^2\right]\psi = E\psi \qquad (6)$$

As demonstrated above (eqn 3) the relativistic energy operator is a 4x4 matrix. Therefore, the wave function must be a four-component vector.

At this point Sherwin turns to the example of the free particle in the x-direction (see pages 292-295). He assumes that the solution has the form of a plane wave. However, as shown below substitution of the deBroglie equation in the plane wave equation yields the momentum eigenfunction in coordinate space.

$$\exp\left(i\frac{2\pi}{\lambda}x\right) \xrightarrow{\lambda = h/p} \exp\left(i\frac{px}{\hbar}\right)$$

This means that this problem is extremely easy to solve in momentum space where the momentum operator is multiplicative. The calculation of the energy eigenvalues is straight forward using **Mathcad's *eigenvals*** command. We simply ask for the eigenvalues of the relativistic energy operator as shown below.

$$eigenvals\left[-c\cdot\left(\alpha_x\cdot p_x + \beta\cdot m\cdot c\right)\right] \rightarrow \begin{pmatrix} c\cdot\sqrt{c^2\cdot m^2 + p_x{}^2} \\ c\cdot\sqrt{c^2\cdot m^2 + p_x{}^2} \\ -c\cdot\sqrt{c^2\cdot m^2 + p_x{}^2} \\ -c\cdot\sqrt{c^2\cdot m^2 + p_x{}^2} \end{pmatrix}$$

Calculation of the (unnormalized) eigenvectors is equally easy.

$$eigenvecs\left[-c\cdot\left(\alpha_x\cdot p_x + \beta\cdot m\cdot c\right)\right] = \begin{pmatrix} \frac{W + m\cdot c^2}{p_x\cdot c} & 0 & 0 & \frac{-W + m\cdot c^2}{p_x\cdot c} \\ 0 & \frac{W + m\cdot c^2}{p_x\cdot c} & \frac{-W + m\cdot c^2}{p_x\cdot c} & 0 \\ 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix} \quad W = \sqrt{p_x{}^2\cdot c^2 + m^2\cdot c^4}$$

V. Dirac Notation - Analogies with vectors and matrices

Tutorial: *Libre Text Physics*, Graeme Ackland, U. of Edinburg: 1.7: Dirac Notation - Analogies with vectors and matrices

Dirac notation is a shorthand for integrals, for example **the overlap** between two wavefunctions can be written as:

$\langle\chi|\phi\rangle$ instead of $\int\int\int \chi^*(\mathbf{r})\phi(\mathbf{r})d^3\mathbf{r}$.

Note: $|\psi\rangle = \sum_n |n\rangle\langle n|\psi\rangle$ is a linear superposition in the discrete (rather than continuous) basis set $\{|n\rangle\}$.

(Where d^3r is the **scalar volume element**, sometimes called $r^2\sin\theta\, d\theta d\phi dr$, $dxdydz$, dV, or $d\tau$)

But also if we have a **complete set of orthonormal basis states *i***, the **overlap** is also the sum of the overlaps between each *i* and χ and ϕ

$$\langle\chi|\phi\rangle = \sum_i \langle\chi|i\rangle\langle i|\phi\rangle$$

A summation convention is also sometimes used, such that when a state symbol appears twice, first as a ket, then as a bra, it is assumed to be summed over a complete set of orthonormal basis states. The expression above is then further abbreviated to $\langle\chi|i\rangle\langle i|\phi\rangle$. This convention can be confusing.

Compare this with the vector dot product formula $b\cdot a = b_x\cdot a_x + b_y\cdot a_y + b_z\cdot a_x = \sum_i \left[\left(b\cdot e_i\right)\cdot\left(e_i\cdot a\right)\right]$

where e_i are the unit vectors in x, y and z directions. Just as any vector can be expressed as a linear combination of $\mathbf{e_i}$, so any quantum state can be expressed as **a linear combination of basis states i**. There are certain conditions on the basis states, e.g. they must be 'orthonormal' $\langle j|i\rangle = \delta_{ij}$ just as $e_i.e_j = \delta_{ij}$. Just as the three Cartesian vectors span a three dimensional space, so the many **basis states span a many-dimensional space**. In some cases (e.g. Fourier expansions, hydrogen wavefunctions) there are an infinite number of basis states which are therefore related to spanning an infinite-dimensional space. Mathematicians call these 'Hilbert spaces'. Any state ϕ can thus be viewed as a vector in a multi-dimensional space, where **each dimension** corresponds to **one of the basis functions**. It is thus common to use the words eigenstate and eigenvector interchangeably to refer to $|\phi\rangle$

Even before the discovery of quantum mechanics, mathematicians had solved many of the problems in this area. **In Dirac notation** we have **two quantities**, the bra and the ket, whereas in vector algebra we have only one, this is because there is not an exact analogy to commutation for Dirac brackets: $\langle\chi|\phi\rangle = \langle\phi|\chi\rangle^*$ includes taking a **complex conjugate**. Consider manipulating the bras and kets. We can write a vector in terms of its components thus

$$A = \sum_i \left[e_i\cdot\left(e_i\cdot A\right)\right]$$

where $(e_i.A)$ is the amount of $\mathbf{A}$ along the e_i axis; the components. The quantities on either side of the equation are not numbers but **vectors**. We can generate a whole algebra based on vectors. Likewise we can write a state thus: $|\phi\rangle = \sum |i\rangle\langle i|\phi\rangle$ where $\langle i|\phi\rangle$ **is the amount of ϕ along the *i* basis state**; the components or expansion coefficients. The quantities on each side of this equation are not numbers but **functions**. ϕ is a normalized wavefunction iff $\sum |\langle i|\phi\rangle|^2 = 1$. We can then generate a whole algebra based on bras and kets.

For any different complete sets of basis states *i* and *j*, we can write: $|\phi\rangle = \sum |j\rangle\langle j|\phi\rangle$, and $|\phi\rangle = \sum |i\rangle\langle i|\phi\rangle$.

Expansions in *i* and *j* are called different **representations** of ϕ. This is very similar to using different coordinate systems: the bases *i* and *j* are **analogous to two sets of axes rotated with respect to one another**. We might choose complete set of wavefunctions as a representation which includes ϕ, just as we sometimes choose axes such that some special vector points along the z -axis.

Going even further, the expansion in a basis can be done for any $|\phi\rangle$, so we can dispense with $|\phi\rangle$ and write:

$\mathbf{1} = \sum |i\rangle\langle i|$, the unit operator

All this means is that **in any equation** you can always proceed by breaking the states down into a **complete, orthonormal set of basis functions.**

Hilbert Space: We can represent a qubit as a **Two-Dimensional Complex Hilbert space, C^2**. **A quantum state is a ray in Hilbert space.** The state of the qubit at any given time can be represented **by a vector** in this complex Hilbert space. A qubit system of say 100 qubits can handle 2^{100} states.
Relative phases of waveforms (states) are of fundamental importance for quantum algorithms in that they allow for constructive interference and destructive interference.
Qubits are abstract mathematical objects with certain specific properties.

With regard to QC, it should be noted that Quantum Mechanics or Matrix Mechanics is not Quantum Physics. Rather, it is the collection of mathematical tools used to analyze physical systems which are, to the best of anyone's ability to test, known to behave according to the laws of quantum physics.

Just as a classical bit has a state – either 0 or 1, a qubit also has a state. Two possible states for a qubit are the states $|0\rangle$ and $|1\rangle$, which correspond to the states 0 and 1 for a classical bit. Notation like ' $|\ \rangle$ ' is called the *Dirac notation*. The difference between bits and qubits is that **a qubit can be in a state other than $|0\rangle$ or $|1\rangle$.**
It is **also possible to form linear combinations of states**, often called **superpositions**:

$$|\Psi\rangle = \alpha\,|0\rangle + \beta\,|0\rangle$$

In the Dirac notation, the symbol identifying **a vector** is written inside a 'ket', and looks like $|\,a\,\rangle$. We denote the **dual vector** for a (defined later) with a 'bra', written as $\langle\,a\,|$. Then **inner vector products** will be written as 'bra-kets' (e.g. $\langle a\,|\,b\,\rangle$). While bras and kets are both elements of vector spaces, they are **elements of different vector spaces**. The ket corresponds to the normal vectors while the **bra corresponds to a covector.** Kets are part of one vector space while **bras are part of the corresponding dual vector space.**

The numbers a and ß are complex numbers, although for many purposes not much is lost by thinking of them as real numbers. Put another way, the state of a qubit is a *vector in a **two-dimensional complex vector space***. The special states $|\,0\,\rangle$ and $|\,1\,\rangle$ are known as *computational basis states*, and form an ***orthonormal basis*** for this vector space. We can examine a bit to determine whether it is in the state 0 or 1. Rather remarkably, **we *cannot examine a qubit to determine its quantum state***, that is, the values of a and ß. Instead, quantum mechanics tells us that we can *only acquire much more restricted information* about the quantum state. When we measure a qubit we get either the result 0, with probability $|a|^2$, or the result 1, with probability $|ß|^2$. Naturally $|a|^2 + |ß|^2 = 1$, since the probabilities must sum to one. Thus, in general **a qubit's state is a *unit vector in a two-dimensional complex vector space*.** This dichotomy between the unobservable state of a qubit and the observations we can make lies at the heart of quantum computation and quantum information. A qubit can **exist in a continuum of states between $|0\rangle$ and $|1\rangle$**, until it is observed. When a qubit is measured, it only ever gives '0' or '1' as the measurement result – probabilistically. Because $|a|^2 + |ß|^2 = 1$, we may write this as (**See Section VIII**.)

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

where **θ, ϕ and γ** are real numbers. We can ignore the phase factor of $e^{iγ}$ out the front, because it has no observable effects. The numbers θ and ϕ define a point on the unit three-dimensional complex sphere, as shown in Section V.

This sphere is often called the Bloch sphere; it provides a useful means of visualizing the state of a **single qubit**. How much information is represented by a qubit? Paradoxically, there are an infinite number of points on the unit sphere.

A **bra-ket pair** can be thought of as a **vector projection** (i.e., a dot product) - the projection of the content of the ket onto the content of the bra, or the "**shadow" the ket casts on the bra.** Example, $\langle\Phi|\psi\rangle$ is projection of state ψ onto state Φ. It is the amplitude (probability amplitude) that a system in state $|\psi\rangle$ will be subsequently found in state $|\Phi\rangle$

Suppose we have two qubits. **A two qubit system** has **four computational basis states** denoted $|00>$, $|01>$, $|10>$, and $|11>$. A pair of qubits can also exist in superpositions of these four states, so the quantum state of two qubits involves associating a complex coefficient, sometimes called an amplitude, with each computational basis state, such that the state vector describing the two qubits is

$$|\psi\rangle = \alpha_{00}|00\rangle + \alpha_{01}|01\rangle + \alpha_{10}|10\rangle + \alpha_{11}|11\rangle$$

Important **2 bit states** are the 4 Bell states, e.g.: $\frac{|00\rangle + |11\rangle}{\sqrt{2}}$

Dirac notation is a succinct and powerful language for expressing quantum mechanical principles; in some of our examples that follow, restricting attention to one-dimensional examples reduces the possibility that mathematical complexity will stand in the way of understanding. Quantum Mechanics texts make extensive use of Dirac notation.

Wave-particle duality is the essential concept of quantum mechanics. In 1924 Louis De Broglie expressed this idea mathematically as $\lambda = h/mv = h/p$. On the left is the wave property , and on the right the particle property mv, its momentum. The most general **coordinate space wavefunction for a free particle with wavelength** is the complex Euler function shown below.

$$\langle x|\lambda\rangle = \exp\left(i2\pi\frac{x}{\lambda}\right) = \cos\left(2\pi\frac{x}{\lambda}\right) + i\sin\left(2\pi\frac{x}{\lambda}\right)$$

Feynman called this equation "*the most remarkable formula in mathematics*." He referred to it as "our jewel." And indeed it is, because when it is enriched with de Broglie's relation it serves as the foundation of quantum mechanics.

According to de Broglie's hypothesis, a particle with a well-defined wavelength also has a well-defined momentum. Therefore, we can obtain the momentum wavefunction (unnormalized) of the particle in coordinate space by substituting the deBroglie relation into Equation $\langle x|p\rangle = \exp\left(\frac{ipx}{\hbar}\right)$

.Quantum mechanics teaches that **the wavefunction contains all the physical information about a system** that can be known, and that **one extracts information** from the wavefunction **using quantum mechanical operators**. There is, therefore, **an operator for each observable property.**
For example, in momentum space if a particle has a well-defined momentum we write its state as $|p>$. If we operate on this state with the momentum operator $\hat{p}$, the following eigenvalue equation is satisfied.

$$\hat{p}|p\rangle = p|p\rangle$$

We say the system is in a state which is an eigenfunction of the momentum operator $\hat{p}$ with eigenvalue p. In other words, operating on the momentum eigenfunction with the momentum operator, in momentum space, returns the momentum eigenvalue times the original momentum eigenfunction. From $\lambda = h/mv = h/p$ λ ν

The state space in quantum mechanics is a complex finite or infinite vector space. Dirac denotes an element f of the vector space by $|f>$, which he then calls a ket vector. An example for a one-dimensional ket is Schrödinger's wave function $|\psi>$, whose representation in position space is the well-known complex-valued wave function $\psi(x)$. An example for a four-dimensional ket is the vector

$$|\psi\rangle \stackrel{\text{def}}{=} \psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix}$$

We then define a dual to each ket called the bra. We get a bra from the respective ket by taking its conjugate complex (if the ket is a vector, we also need to transpose):

$$\langle f| \stackrel{\text{def}}{=} (f^*)^\intercal = f^\dagger$$

Note that the ket $|\psi>$ stands for the entire wave function ψ.
The scalar product of two vectors can then be written with the bra and the ket as

$$\langle f| \stackrel{\text{def}}{=} (f^*)^\intercal = f^\dagger \qquad \text{we then have} \qquad \langle f|g\rangle = \langle g|f\rangle^*$$

VI. Vector and Matrix Math

Products of ket and bra-Spin vectors

Note: *The **arrow symbol** → below is used in Mathcad to evaluate an expression symbolically. Mathcad returns the result as another expression in terms of the variable and symbols in the original problem.*

Vector Inner Product:

$$\begin{pmatrix} a & b \end{pmatrix} \cdot \begin{pmatrix} c \\ d \end{pmatrix} \rightarrow a \cdot c + b \cdot d$$

Vector Outer Product:

$$\begin{pmatrix} c \\ d \end{pmatrix} - (ab) \rightarrow \begin{pmatrix} a \cdot c & b \cdot c \\ a \cdot d & b \cdot d \end{pmatrix}$$

$$tr\left[\begin{pmatrix} c \\ d \end{pmatrix} \cdot \begin{pmatrix} a & b \end{pmatrix}\right] \rightarrow a \cdot c + b \cdot d$$

$$|\uparrow\rangle\langle\uparrow| \quad UpUp := \begin{pmatrix} 1 \\ 0 \end{pmatrix} \cdot \begin{pmatrix} 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

$$|\uparrow\rangle\langle\downarrow| \quad UpDn := \begin{pmatrix} 1 \\ 0 \end{pmatrix} \cdot \begin{pmatrix} 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

$$|\downarrow\rangle\langle\uparrow| \quad DnUp := \begin{pmatrix} 0 \\ 1 \end{pmatrix} \cdot \begin{pmatrix} 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

$$|\downarrow\rangle\langle\downarrow| \quad DnDn := \begin{pmatrix} 0 \\ 1 \end{pmatrix} \cdot \begin{pmatrix} 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

Matrix-Vector Product:

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \cdot \begin{pmatrix} x \\ y \end{pmatrix} \rightarrow \begin{pmatrix} a \cdot x + b \cdot y \\ c \cdot x + d \cdot y \end{pmatrix}$$

$$\begin{pmatrix} x & y \end{pmatrix} \cdot \begin{pmatrix} a & b \\ c & d \end{pmatrix}^T \rightarrow \begin{pmatrix} a \cdot x + b \cdot y & c \cdot x + d \cdot y \end{pmatrix}$$

Expectation Value:

$$\begin{pmatrix} x & y \end{pmatrix} \cdot \begin{pmatrix} a & b \\ c & d \end{pmatrix} \cdot \begin{pmatrix} x \\ y \end{pmatrix} \rightarrow a \cdot x^2 + d \cdot y^2 + b \cdot x \cdot y + c \cdot x \cdot y$$

$$\begin{pmatrix} x & y \end{pmatrix} \cdot \begin{pmatrix} a & b \\ c & d \end{pmatrix}^T \cdot \begin{pmatrix} x \\ y \end{pmatrix} \rightarrow x \cdot \left(a \cdot x + b \cdot y\right) + y \cdot \left(c \cdot x + d \cdot y\right)$$

$$\mathrm{tr}\left[\begin{pmatrix} x \\ y \end{pmatrix} \cdot \begin{pmatrix} a & b \\ c & d \end{pmatrix}\right] \rightarrow a \cdot x^2 + d \cdot y^2 + b \cdot x \cdot y + c \cdot x \cdot y$$

$$tr\left[\begin{pmatrix} a & b \\ c & d \end{pmatrix} \cdot \begin{pmatrix} x \\ y \end{pmatrix} \cdot \begin{pmatrix} x & y \end{pmatrix}\right] \rightarrow a \cdot x^2 + d \cdot y^2 + b \cdot x \cdot y + c \cdot x \cdot y$$

Matrix Product:

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \cdot \begin{pmatrix} w & x \\ y & z \end{pmatrix} \rightarrow \begin{pmatrix} a \cdot w + b \cdot y & a \cdot x + b \cdot z \\ c \cdot w + d \cdot y & c \cdot x + d \cdot z \end{pmatrix}$$

Vector Tensor Product, ⊗:

$$\begin{pmatrix} a \\ b \end{pmatrix} \otimes \begin{pmatrix} c \\ d \end{pmatrix} = \begin{pmatrix} a \begin{pmatrix} c \\ d \end{pmatrix} \\ b \begin{pmatrix} c \\ d \end{pmatrix} \end{pmatrix} = \begin{pmatrix} ac \\ ad \\ bc \\ bd \end{pmatrix}$$

$$VTP(V_1, V_2) := \begin{pmatrix} V1_0 \cdot V2_0 \\ V1_0 \cdot V2_1 \\ V1_1 \cdot V2_0 \\ V1_1 \cdot V2_1 \end{pmatrix} \qquad VTP\left[\begin{pmatrix} a \\ b \end{pmatrix}, \begin{pmatrix} c \\ d \end{pmatrix}\right] \rightarrow \begin{pmatrix} a \cdot c \\ a \cdot d \\ b \cdot c \\ b \cdot d \end{pmatrix}$$

kronecker(M, N) Multiplies matrix N by each element of matrix M, returning an M•N by M•N array.
Arguments: M and N are square matrices.

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \otimes \begin{pmatrix} w & x \\ y & z \end{pmatrix} = \begin{pmatrix} a\begin{pmatrix} w & x \\ y & z \end{pmatrix} & b\begin{pmatrix} w & x \\ y & z \end{pmatrix} \\ c\begin{pmatrix} w & x \\ y & z \end{pmatrix} & d\begin{pmatrix} w & x \\ y & z \end{pmatrix} \end{pmatrix} = \begin{pmatrix} aw & ax & bw & bx \\ ay & az & by & bz \\ cw & cx & dw & dx \\ cy & cz & dy & dz \end{pmatrix}$$

Pauli Spin Matrices

$$X := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$Z := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$MTP(A, B) := \begin{pmatrix} A_{0,0}\cdot B_{0,0} & A_{0,0}\cdot B_{0,1} & A_{0,1}\cdot B_{0,0} & A_{0,1}\cdot B_{0,1} \\ A_{0,0}\cdot B_{1,0} & A_{0,0}\cdot B_{1,1} & A_{0,1}\cdot B_{1,0} & A_{0,1}\cdot B_{1,1} \\ A_{1,0}\cdot B_{0,0} & A_{1,0}\cdot B_{0,1} & A_{1,1}\cdot B_{0,0} & A_{1,1}\cdot B_{0,1} \\ A_{1,0}\cdot B_{1,0} & A_{1,0}\cdot B_{1,1} & A_{1,1}\cdot B_{1,0} & A_{1,1}\cdot B_{1,1} \end{pmatrix}$$

$$kronecker(X, Z) = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}$$

$$S_x := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$MTP\left[\begin{pmatrix} a & b \\ c & d \end{pmatrix}, \begin{pmatrix} w & x \\ y & z \end{pmatrix}\right] \rightarrow \begin{pmatrix} a\cdot w & a\cdot x & b\cdot w & b\cdot x \\ a\cdot y & a\cdot z & b\cdot y & b\cdot z \\ c\cdot w & c\cdot x & d\cdot w & d\cdot x \\ c\cdot y & c\cdot z & d\cdot y & d\cdot z \end{pmatrix}$$

$$MTP(X, Z) = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}$$

Matrix Eigenvalues and Eigenvectors (unnormalized):

$$eigenvals\left(\begin{pmatrix} a & b \\ b & a \end{pmatrix}\right) \rightarrow \begin{pmatrix} a-b \\ a+b \end{pmatrix}$$

$$MTP(S_x, S_x) = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

$$\left|\begin{pmatrix} a-\lambda & b \\ b & a-\lambda \end{pmatrix}\right| = 0 \text{ solve}, \lambda \rightarrow \begin{pmatrix} a+b \\ a-b \end{pmatrix}$$

$$\begin{pmatrix} -1 & 1 \\ 1 & 1 \end{pmatrix}^{-1} \cdot \begin{pmatrix} a & b \\ b & a \end{pmatrix} \cdot \begin{pmatrix} -1 & 1 \\ 1 & 1 \end{pmatrix} \rightarrow \begin{pmatrix} a-b & 0 \\ 0 & a+b \end{pmatrix}$$

$$eigenvecs\left(\begin{pmatrix} a & b \\ b & a \end{pmatrix}\right) \rightarrow \begin{pmatrix} -1 & 1 \\ 1 & 1 \end{pmatrix}$$

$$\begin{pmatrix} a & b \\ b & a \end{pmatrix} \cdot \begin{pmatrix} x \\ y \end{pmatrix} = (a-b) \cdot \begin{pmatrix} x \\ y \end{pmatrix} \text{ solve}, y \rightarrow -x \qquad \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} -1 \\ 1 \end{pmatrix}$$

$$\begin{pmatrix} a & b \\ b & a \end{pmatrix} \cdot \begin{pmatrix} x \\ y \end{pmatrix} = (a+b) \cdot \begin{pmatrix} x \\ y \end{pmatrix} \text{ solve}, y \rightarrow x \qquad \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

Completeness Relations:

$$\text{Black} \cdot \text{Black}^T + \text{White} \cdot \text{White}^T = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\text{Hard} \cdot \text{Hard}^T + \text{Soft} \cdot \text{Soft}^T = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Tensor Products of Vector Spaces, Math ⊗

Mathcad uses the matrix operation "kronecker ()" to calculate a Tensor Product, ⊗

The Mathcad syntax for tensor multiplication of TWO 2-dimensional vectors. ⊗

$$\psi(a,b) := submatrix(kronecker(augment(a,n),augment(b,n)),1,4,1,1)$$

The Mathcad syntax for tensor multiplication of THREE 2-dimensional vectors. ⊗

$$\psi(a,b,c) := submatrix(kronecker(augment(a,n),kronecker(augment(b,n),augment(c,n))),1,8,1,1)$$

kronecker(M, N)
Multiplies matrix N by each element of matrix M, returning an M•N by M•N array.
Arguments: M and N are square matrices.

The Tensor Product of Matrices is also defined as:

$$A = \begin{pmatrix} a_{11} & \dots & a_{1n} \\ \vdots & & \vdots \\ a_{n1} & \dots & a_{nn} \end{pmatrix} \quad B = \begin{pmatrix} b_{11} & \dots & b_{1m} \\ \vdots & & \vdots \\ b_{m1} & \dots & b_{mm} \end{pmatrix} \qquad A \otimes B = \begin{pmatrix} a_{11}B & \dots & a_{1n}B \\ \vdots & & \vdots \\ a_{n1}B & \dots & a_{nn}B \end{pmatrix}$$

and A ⊗ B is therefore a matrix of degree mn.

Tutorial: *QUANTUM COMPUTING Gentle Introduction*, Eleanor Rieffel, Page 33

The *tensor product* $V \otimes W$ of two vector spaces V and W with bases $A = \{|\alpha_1\rangle, |\alpha_2\rangle, \dots, |\alpha_n\rangle\}$ and $B = \{|\beta_1\rangle, |\beta_2\rangle, \dots, |\beta_m\rangle\}$ respectively is an nm-dimensional vector space with a basis consisting of the nm elements of the form $|\alpha_i\rangle \otimes |\beta_j\rangle$ where $\otimes$ is the tensor product, an abstract binary operator that satisfies the following relations:

$$(|v_1\rangle + |v_2\rangle) \otimes |w\rangle = |v_1\rangle \otimes |w\rangle + |v_2\rangle \otimes |w\rangle$$

$$|v\rangle \otimes (|w_1\rangle + |w_2\rangle) = |v\rangle \otimes |w_1\rangle + |v\rangle \otimes |w_2\rangle$$

$$(a|v\rangle) \otimes |w\rangle = |v\rangle \otimes (a|w\rangle) = a(|v\rangle \otimes |w\rangle).$$

Taking $k = \min(n, m)$, all elements of $V \otimes W$ have form

$$|v_1\rangle \otimes |w_1\rangle + |v_2\rangle \otimes |w_2\rangle + \cdots + |v_k\rangle \otimes |w_k\rangle$$

for some $v_i \in V$ and $w_i \in W$. Due to the relations defining the tensor product, such a representation is not unique. Furthermore, while all elements of $V \otimes W$ can be written

$$\alpha_1(|\alpha_1\rangle \otimes |\beta_1\rangle) + \alpha_2(|\alpha_2\rangle \otimes |\beta_1\rangle) + \cdots + \alpha_{nm}(|\alpha_n\rangle \otimes |\beta_m\rangle),$$

most elements of $V \otimes W$ cannot be written as $|v\rangle \otimes |w\rangle$, where $v \in V$ and $w \in W$. It is common to write $|v\rangle|w\rangle$ for $|v\rangle \otimes |w\rangle$.

QUANTUM COMPUTING EXPLAINED, David McMahon

Tensor Products - Chapter 4

In quantum mechanics we don't always work with single particles in isolation. In many cases, some of which are seen in the context of quantum information processing, it is necessary to work with multiparticle states. Mathematically, to understand multiparticle systems in quantum mechanics, it is necessary to be able to construct a Hilbert space H that is a composite of the independent Hilbert spaces that are associated with each individual particle. The machinery required to do this goes by the name of the Kronecker or tensor product. We consider the two-particle case. Suppose that H_1 and H_2 are two Hilbert spaces of dimension N_1 and N_2. We can put these two Hilbert spaces together to construct a larger Hilbert space. We denote this larger space by H and use the tensor product operation symbol $\otimes$. So we write $H = H_1 \otimes H_2$

The dimension of the larger Hilbert space is the product of the dimensions of H_1 and H_2. Once again, we assume that $\dim(H_1) = N_1$ and $\dim(H_2) = N_2$. Then $\dim(H) = N_1 N_2$
Next we start getting down to business and learn how to represent state vectors in the composite Hilbert space.

REPRESENTING COMPOSITE STATES IN QUANTUM MECHANICS

A state vector belonging to H is the tensor product of state vectors belonging to H_1 and H_2. We will show how to represent such vectors explicitly in a moment. For now we will just present some notation, sticking to the more abstract Dirac notation. Let $|\varphi\rangle \in H_1$ and $|\chi\rangle \in H_2$ be two vectors that belong to the Hilbert spaces used to construct H . We can construct a vector $|\psi\rangle \in H$ using the tensor product in the following way:

$$|\psi\rangle = |\phi\rangle \otimes |\chi\rangle$$

The tensor product of two vectors is linear. That is,

$$|\phi\rangle \otimes [|\chi_1\rangle + |\chi_2\rangle] = |\phi\rangle \otimes |\chi_1\rangle + |\phi\rangle \otimes |\chi_2\rangle$$
$$[|\phi_1\rangle + |\phi_2\rangle] \otimes |\chi\rangle = |\phi_1\rangle \otimes |\chi\rangle + |\phi_2\rangle \otimes |\chi\rangle$$

Moreover the tensor product is linear with respect to scalars

$$|\phi\rangle \otimes (\alpha|\chi\rangle) = \alpha|\phi\rangle \otimes |\chi\rangle$$

and vice versa. To construct a basis for the larger Hilbert space, we simply form the tensor products of basis vectors from the spaces H_1 and H_2. Let us denote the basis of H_1 by $|u_i\rangle$ and the basis of H_2 by $|v_i\rangle$. Then it follows that we can construct a basis $|w_i\rangle$ for $H = H_1 \otimes H_2$ using $|w_i\rangle = |u_i\rangle \otimes |v_i\rangle$
Note that the order of the tensor product is not relevant, meaning

$$|\phi\rangle \otimes |\chi\rangle = |\chi\rangle \otimes |\phi\rangle$$

It is often cumbersome to write the $\otimes$ symbol. Therefore you should be aware that the tensor product $|\varphi\rangle \otimes |\chi\rangle$ is often written more simply as $|\varphi\rangle|\chi\rangle$, or even as $|\varphi\chi\rangle$.

Quantum Bit and Quantum Register, *Fundamentals of Quantum Information*, Sagawa & Yoshida, Chap. 8

The qubit (quantum bit) can be implemented by any quantum system with two states. For example, the spin-up |↑> and the spin-down |↓> states of electrons can be assigned to | 0 > and | 1 > (see Bloch Sphere Section). **The set of qubits** is called the quantum register, or simply the register. An integer 6 is expressed as 110 in the binary system. In the quantum register, this can be represented as a direct product of **three states**, $|6\rangle = |1\rangle \otimes |1\rangle \otimes |0\rangle$
The state can be implemented by a three-bit register.
In general, a number of n-bits

$$a = 2^{n-1}a_{n-1} + 2^{n-2}a_{n-2} + \cdots + 2^0 a_0$$

can be expressed by a state of n-bit register,

$$|a\rangle = |a_{n-1}\rangle \otimes |a_{n-2}\rangle \otimes \cdots \otimes |a_1\rangle \otimes |a_0\rangle \equiv |a_{n-1}a_{n-2}\cdots a_1 a_0\rangle.$$

where ⊗ is the tensor product. See Section VI.

A quantum state of the n-bit register can be generalized to be a linear combination of states with numbers from a = 0 to a = $2^n - 1$:

Using the principles of quantum mechanics, **we can construct new types of reversible (unitary) gates which do not exist in the classical gates.** The Hadamard transformation H, for example, performs the operation,

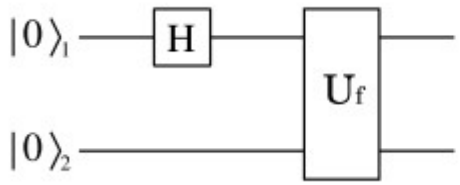
$$H|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \qquad \sigma_z := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$H|1\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle). \qquad D_i^s(\alpha) = \cos\left(\frac{\alpha}{2}\right)\mathbf{1} - i\sin\left(\frac{\alpha}{2}\right)\sigma_i$$

This gate is implemented by the product of the spin-rotation operator $D_y^s\left(\frac{\pi}{2}\right)$ and the spin operator σ_z.

$$H = D_y^s\left(\frac{\pi}{2}\right)\sigma_z = \left(\cos\left(\frac{\pi}{4}\right)\mathbf{1} - i\sin\left(\frac{\pi}{4}\right)\sigma_y\right)\sigma_z = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

The rotation of spin can be achieved by the magnetic field such as the experimental set-up of Stern and Gerlach. Many quantum algorithms are based on so called quantum parallelism. As an defective algorithm by the quantum parallelism, we will show that the quantum computer can calculate the function f(x) for many different values of x by one instruction. As a simple example, let us take the function f(x), x ∈ {0,1}, f ∈ {0,1}, where both x and f(x) have 1 bit size. We apply f(x) to the state |x,y> with two registers x and y. The first register x is called the data register while the second register y is called the target register. The operator U_f acts on the state | x,y> as $U_f|x,y\rangle = |x, y \oplus f(x)\rangle$
where y ⊗ f(x) means the logical sum with mod 2. The operator U_f is called the Oracle operator or "the black box."



$$|\psi\rangle = \frac{|0, f(0)\rangle + |1, f(1)\rangle}{\sqrt{2}}$$

We apply first the Hadamard transformation to the state | 0> of the data register. Secondly we apply U_f to obtain the state

$$|\psi\rangle = U_f H|0,0\rangle = U_f \frac{1}{\sqrt{2}}\{|0,0\rangle + |1,0\rangle\}$$
$$= \frac{1}{\sqrt{2}}\{|0, f(0)\rangle + |1, f(1)\rangle\}$$

The state arises as a result by the algorithm based on the **quantum parallelism**; the state $|\psi>$ **contains two results f(0) and f(1) as a linear combination**. This is the fundamental difference from the parallelism in the classical computer. In the parallelism in the classical circuits, the different values of f(x) are calculated in separate circuits. In the quantum parallelism, on the other hand, all the values of f(x) are calculated in a single circuit. The concept of the quantum parallelism holds not only with a single bit but also with n data bits. Let us write $H^{\otimes n}$ to express the Hadamard transformation acting on each bit of the n bit state $|0>^{\otimes n} = |00\cdots0>$. Then we have a linear combination of 2^n states: $|\psi\rangle = H^{\otimes n}|0\rangle = H \otimes H \otimes \cdots \otimes H|00\cdots0\rangle$ where $\otimes$ is the tensor product.

$$
\begin{aligned}
&= \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes \cdots \otimes \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \\
&= \frac{1}{\sqrt{2^n}}(|00\cdots0\rangle + |00\cdots1\rangle + \cdots + |11\cdots1\rangle) \\
&= \frac{1}{\sqrt{2^n}} \sum_{x=0}^{2^n-1} |x\rangle. \qquad (8.12)
\end{aligned}
$$

The above result shows that a **single operation of U_f** produces a state which **contains all of the 2^n values of the function f(x).** This conclusion is based on nothing but the principles of quantum mechanics. However when we consider the problem of quantum mechanical measurement, it is not very clear how effective the quantum parallelism is compared with the classical parallelism. In reality, the output register f(x) is determined by the observation of value x in the input register. This procedure implies that one output is determined by one input data just like the classical computer.

Two Different Formulations of Quantum Mechanics

Schrödinger's Wave Mechanics Formulation

Schrödinger's equation for the one-dimensional harmonic oscillator will be set up in both coordinate and momentum space using the information in the table. Schrödinger's equation is the quantum mechanical energy eigenvalue equation, and for the harmonic oscillator it looks like this initially, the information in the table. Schrödinger's equation is the quantum mechanical energy eigenvalue equation, and for the harmonic oscillator it looks like this initially,

$$\left[\frac{\hat{p}^2}{2m} + \frac{1}{2}k\hat{x}\right]|\Psi\rangle = E|\Psi\rangle$$

Energy observables: Hamiltonian in Sch. Eq. gives the time evolution of any system. Sch. Equation is the energy eigenvalue equation.

$$\hat{H}|E\rangle = E\,|E\rangle$$

The term in brackets on the left is the classical energy written as an operator without a commitment to a representation (position or momentum) for the calculation. See Sections **XXI and XXII** for solutions to the Schrödinger's equation. It is now necessary to explore the meaning of $<x|\Psi>$. It is the probability amplitude that a system in the state $|\Psi>$.

There are, of course, many formulations of quantum mechanics, and all of them develop quantum mechanical principles in different ways from diverse starting points, but they are all formally equivalent. In the present approach the key concepts are de Broglie's hypothesis, and the eigenvalue equations expressed in the momentum and coordinate representations, respectively.

Another formulation: Heisenberg or Matrix Mechanics

It identifies the commutation relation of equation as the basis of quantum theory, and adopts operators for position and momentum that satisfy the equation:

$$[\hat{p}, \hat{x}] = \hat{p}\hat{x} - \hat{x}\hat{p} = \frac{\hbar}{i}$$

Quantum mechanics based "exclusively on relationships between quantities that in principle are observable."

This Equation can be confirmed in both coordinate and momentum space for any state function |Ψ> using the matrix operators .

$$\langle x|(\hat{p}\hat{x} - \hat{x}\hat{p})|\Psi\rangle = \frac{\hbar}{i}\left(\frac{d}{dx}x - x\frac{d}{dx}\right)\langle x|\Psi\rangle = \frac{\hbar}{i}\langle x|\Psi\rangle$$

$$\langle p|(\hat{p}\hat{x} - \hat{x}\hat{p})|\Psi\rangle = i\hbar\left(p\frac{d}{dd} - \frac{d}{dp}p\right)\langle p|\Psi\rangle = \frac{\hbar}{i}\langle p|\Psi\rangle$$

The meaning associated with these equations is that the observables associated with **non-commuting operators cannot simultaneously have well-defined values**. This, of course, is just another statement of the **uncertainty principle.**

The famous double-slit experiment illustrates the uncertainty principle in a striking way. To illustrate this it is mathematically expedient to begin with infinitesimally thin slits. Later this restriction will be relaxed. A screen with **infinitesimally thin slits at x_1 and x_2** projects the incident beam into a linear superposition of position eigenstates

$$|\Psi\rangle = \frac{1}{\sqrt{2}}[|x_1\rangle + |x_2\rangle]$$

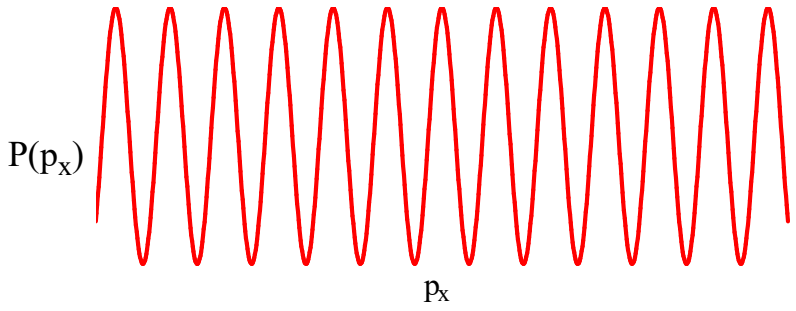
Expressing this state in the coordinate representation yields the following superposition of Dirac delta functions, δ.

$$\langle x|\Psi\rangle = \frac{1}{\sqrt{2}}[\langle x|x_1\rangle + \langle x|x_2\rangle] = \frac{1}{\sqrt{2}}[\delta(x - x_1) + \delta(x - x_2)]$$

According to the uncertainty principle **this localization** of the incident beam in coordinate space is accompanied by a **delocalization** of the x-component of the momentum, p_x. This can be seen by projecting |Ψ> onto momentum space

$$\langle p_x|\Psi\rangle = \frac{1}{\sqrt{2}}[\langle p_x|x_1\rangle + \langle p_x|x_2\rangle] = P(p_x) := \frac{1}{2\sqrt{\pi \cdot h}} \cdot \left(exp\left(-i \cdot p_x \cdot x_1\right) + exp\left(-i \cdot p_x \cdot x_2\right)\right)$$

The momentum probability distribution in the x-direction, $P(p_x) = |\langle p_x|\Psi\rangle|^2$ reveals the required spread in momentum, plus the interesting **interference pattern in the momentum distribution** that will ultimately be projected onto the detection screen. The detection screen is actually measuring the x-component of the momentum.



All nano (atom) sized objects "exist" fundamentally as a Wave-Particle Duality Amplitude

VII. Quantum Superposition

Tutorial: Wikipedia

Quantum superposition is a fundamental principle of quantum mechanics. In classical mechanics, things like position or momentum are always well-defined. We may not know what they are at any given time, but that is an issue of our understanding and not the physical system. In quantum mechanics, a particle can be **in a superposition of different states**. It can be in **two places at once** (see double-slit experiment). A measurement always finds it in one state, but before and after the measurement, it interacts in ways that **can only be explained by having a superposition of different states.**

Mathematically, much like waves in classical physics, any two (or more) quantum states can be added together ("superposed") and the result will be another valid quantum state; conversely, **every quantum state can be represented as a sum of two or more other distinct states.** Mathematically, it refers to a property of solutions to the Schrödinger equation; **since the Schrödinger equation is linear, any linear combination of solutions will also be a solution(s).**

An example of a physically observable manifestation of the wave nature of quantum systems is the interference peaks from an electron beam in a double-slit experiment. The pattern is very similar to the one obtained by diffraction of classical waves.

Another example is a quantum logical qubit state, as used in quantum information processing, **which is a quantum superposition of the "basis states" |0⟩ and |1⟩.** Here **|0⟩** is the Dirac notation for the quantum state that will always give the result **0** when converted to classical logic by a measurement. Likewise |1> is the state that will always convert to **1**. Contrary to a classical bit that can only be in the state corresponding to 0 or the state corresponding to 1, **a qubit may be in a superposition of both states**. This means that the probabilities of measuring 0 or 1 for a qubit are in general neither 0.0 nor 1.0, and multiple measurements made on qubits in identical states will not always give the same result.

Concept

The principle of quantum superposition states that if a physical system may be in many configurations -arrangements of particles or fields—then the **most general state is a combination of all of these possibilities**, where the amount in each configuration is specified by a complex number.

For example, if there are two configurations labeled by 0 and 1, the most general state would be where the coefficients are complex numbers describing how much goes into each configuration. $c_0|0\rangle + c_1|1\rangle$

The principle was described by Paul Dirac as follows:
The general principle of superposition of quantum mechanics applies to the states [that are theoretically possible without mutual interference or contradiction] ... of any one dynamical system. **The original state must be regarded** as the **result of a kind of superposition of the two or more new states**, in a way that cannot be conceived on classical ideas. **Any state** may be considered as the **result of a superposition of two or more other** states, and indeed in an **infinite number of ways**. Conversely, any two or more states may be superposed to give a **new state**. For an equation describing a physical phenomenon, the superposition principle states that a combination of solutions to a linear equation is also a solution of it. When true, the equation is said to obey the superposition principle.

Pure States: The mathematical formulation of quantum mechanics, pure quantum states correspond to **vectors in a Hilbert space**, while **each observable** quantity (such as the energy or momentum of a particle) is **associated with a mathematical operator.** The operator serves as a linear function which acts on the states of the system. **The eigenvalues** of the operator correspond to the **possible values of the observable**.

The superposition principle and the wave function

Exploring the Quantum, Haroche and Raim

The superposition principle and the wave function Let us start by recalling briefly the general framework of quantum theory. Each state of a microscopic system A is represented by a vector in an abstract Hilbert space H_A and the physical observables of this system are associated to Hermitian (self-adjoint) operators in H_A . The linear combination and scalar product of state vectors as well as the operator algebra in H_A are defined in all quantum mechanics textbooks.

The description of the most general state $|\psi\rangle$ of A requires the definition of a reference basis $\{|i\rangle\}$ in H_A, obeying the orthogonality and closure relationships:

$$\langle i \,|j\rangle = \delta_{ij} \; ; \qquad \sum_i |i\rangle \langle i| = \mathbb{1}$$

where δ_{ij} is the usual Kroneker symbol and **1** the unity operator in H_A . The **basis states** are the **eigenstates of a complete ensemble of commuting observables** $O_1, O_2, \ldots, O_k$ which define a 'representation' in H_A .

Once the representation basis is known, any state $|\psi\rangle$ of A is developed as:

$$|\psi\rangle = \mathbb{1}\,|\psi\rangle = \sum_i |i\rangle \langle i \,|\psi\rangle$$

a **linear combination of basis states**, entirely defined by the list of C-number coefficients $c_i = \langle i|\psi\rangle$. A measurement of the complete ensemble $\{O_k\}$ randomly projects $|\psi\rangle$ into one of the $|i|\psi\rangle$ states with the probability $p_i = |c_i|^2$. The $\langle i|\psi\rangle$ scalar product coefficients are thus called 'probability amplitudes'. The normalization of the state ($\langle\psi|\psi\rangle = 1$) ensures that the total probability of all measurement outcomes is equal to 1. Immediately after the **measurement**, the system's state is irreversibly changed,

'jumping' from $|\psi\rangle$ into one of the $|i\rangle$'s.

Repeating the **measurement immediately afterwards** (i.e. before the system has had time to evolve) leaves A with **unit probability** in the **same $|i\rangle$ state**. At this stage, we just enunciate the postulates of the quantum theory of measurement. A description of measurement procedures, which includes a definition of a measuring apparatus and of its coupling with A. We will then try to sharpen our understanding of the irreversible evolution of a quantum system upon measurement, certainly the most difficult aspect of quantum theory.

In everyday language, the above equation, can be loosely expressed by saying that

if a system can exist in different configurations
(corresponding for example to different classical descriptions),
it can also exist in a superposition of these configurations,

so to speak 'suspended' between them. This layman's language is imprecise though, while the above mathematical formula is unambiguous.

The Superposition Principle - Photons - Polarization States, Entanglement

According to the principles of quantum mechanics, systems are set to a definite state only once they are measured. Before a measurement, systems are in an **indeterminate state**; after we measure them, they are in a definite state. If we have a system that can take on one of two discrete states when measured, we can represent the two states in Dirac notation as $|0\rangle$ and $|1\rangle$. We can then represent a **Superposition of States** as a linear combination of these states, such as

$$\frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle$$

Superposition is the linear combination of two or more state vectors is another state vector in the same Hilbert space and describes another state of the system.

As an example, let us consider a property of light that **illustrates a superposition of states**. Light has an intrinsic property called polarization which we can use to illustrate a superposition of states. In almost all of the light we see in everyday life - from the sun, for example - there is no preferred direction for the polarization. **Polarization states can be selected** by means of a polarizing filter, a thin film with an axis that only allows light with polarization parallel to that axis to pass through. With a single polarizing filter, we can **select one** polarization of light, for example *vertical polarization*, which we can denote as $|\uparrow\rangle$. Horizontal polarization, which we can denote as $|\rightarrow\rangle$, is an orthogonal state to vertical polarization. Together, **these states form a basis** for any polarization of light. That is, any polarization state $|\psi\rangle$ can be written as linear combination of these states. We use the Greek letter ψ to denote the state of the system

$$|\psi\rangle = \alpha|\uparrow\rangle + \beta|\rightarrow\rangle$$

The coefficients α and β are complex numbers known as amplitudes. The coefficient α, is associated with vertical polarization and the coefficient β is associated with horizontal polarization. These have an important interpretation in quantum mechanics which we will see in Section VIII.

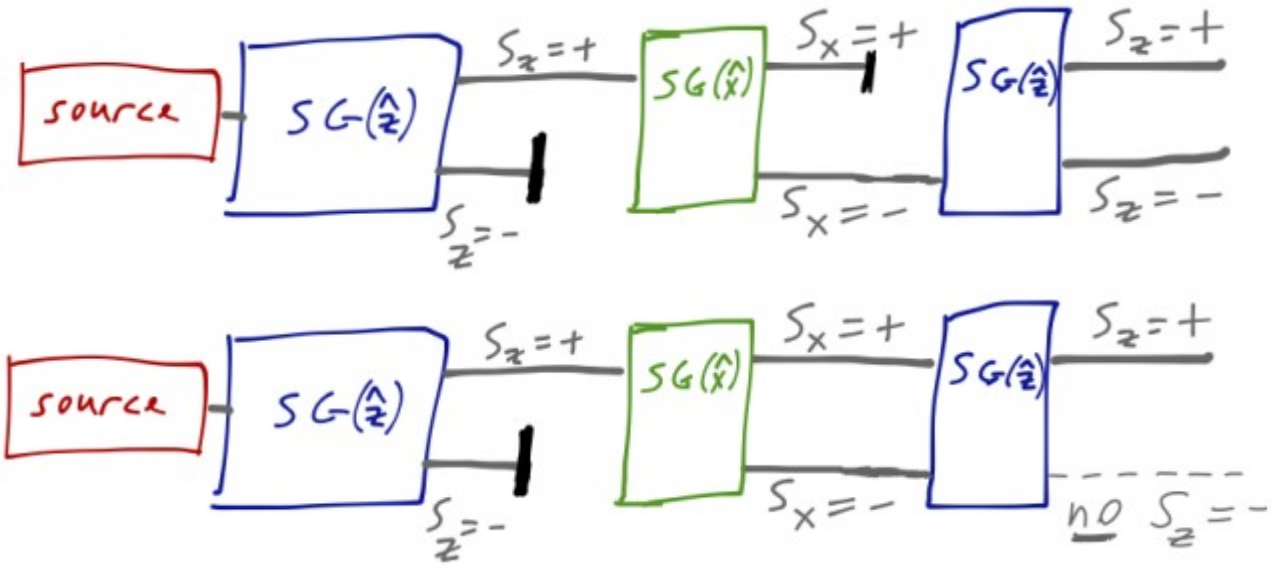
After selecting vertical polarization with a polarizing filter, we can then introduce a **second polarizing filter** after the first. Do you see light? If you answered no to this question, you would be correct. The horizontal state $|\rightarrow\rangle$ is orthogonal to the first, so there is no amount of horizontal polarization after the first vertical filter. Suppose now we oriented the axis of the second polarizing filter at 45°(i.e., along the diagonal ↗ between vertical ↑ and horizontal →) to the first instead of horizontally. Now we ask the same question — would we see any light get through the second filter? If you answered no to this question, you may be surprised to find the answer is yes. We would, in fact, see some amount of light get through the second filter. How could this be if all light after the first filter has vertical polarization? The reason is that **we can express vertical polarization as a superposition of two diagonal components.** That is, letting ↗ denote +45° polarization and ↖ denote -45° polarization, we may write

$$|\uparrow\rangle = \frac{1}{\sqrt{2}}|\nearrow\rangle + \frac{1}{\sqrt{2}}|\nwarrow\rangle$$

It is for this reason that we see some amount of light get past the second filter. Namely, the vertical polarization can be written as a **superposition of states**, one of which is precisely the 45° diagonal state ↗ we are allowing through the second filter. **Since the ↗ state is only one term in the superposition, not all** of the light gets through the filter, but some does. **The amount that gets transmitted is precisely 1/2 in this case.**

Superposition effects are evident when we start chaining them together:

Refer to: https://physicscourses.colorado.edu/phys5250/phys5250_fa19/lecture/lec02-hilbert-spaces/



The *disappearance* of the $S_z = -\hbar/2$ component when we *unblock* the $S_x = +\hbar/2$ output of the middle Stern-Gerlach analyzer is a signature interference effect. Since all of the outputs of this experiment are probabilistic, the statement that the probability observed is different in the "combined" experiment with both outputs unblocked is best written as

$$p(S_z = -|S_x = + \text{ or } S_x = -) \neq p(S_z = -|S_x = +) + p(S_z = -|S_x = -).$$

As I explained last time, this is *suggestive* of superposition, because for any two events A and B in classical probability theory, we have

$$p(A \text{ or } B) = p(A) + p(B) - p(A \text{ and } B).$$

so we can get destructive contributions if we allow the last term. The actual equations that I wrote out last time playing off this relation were not formulated very well, and in particular ignored the very important fact that the state was $S_z = +$ *before* we went through the $SG(\hat{x})$ analyzer - which would lead to some very unwieldy compound conditional probabilities. Besides, we know that in quantum mechanics we work with *probability amplitudes* ψ, which we have to square to get probabilities, schematically

$$p(A) = |\psi(A)|^2$$

so the correct, quantum version of the superposition statement above is

$$p_{\text{quantum}}(A \text{ or } B) = |\psi(A) + \psi(B)|^2 = p(A) + p(B) + 2\text{Re}(\psi^*(A)\psi(B)),$$

In this abstract vector space, passing our beam through a Stern-Gerlach device and blocking one of the output components is exactly a projection along the given direction. It's easy to see in these terms that even after projecting only the $S_z = +\hbar/2$ component out, the subsequent projection on the $S_x = +\hbar/2$ direction will have *both* $\hat{z}$ spin components present.

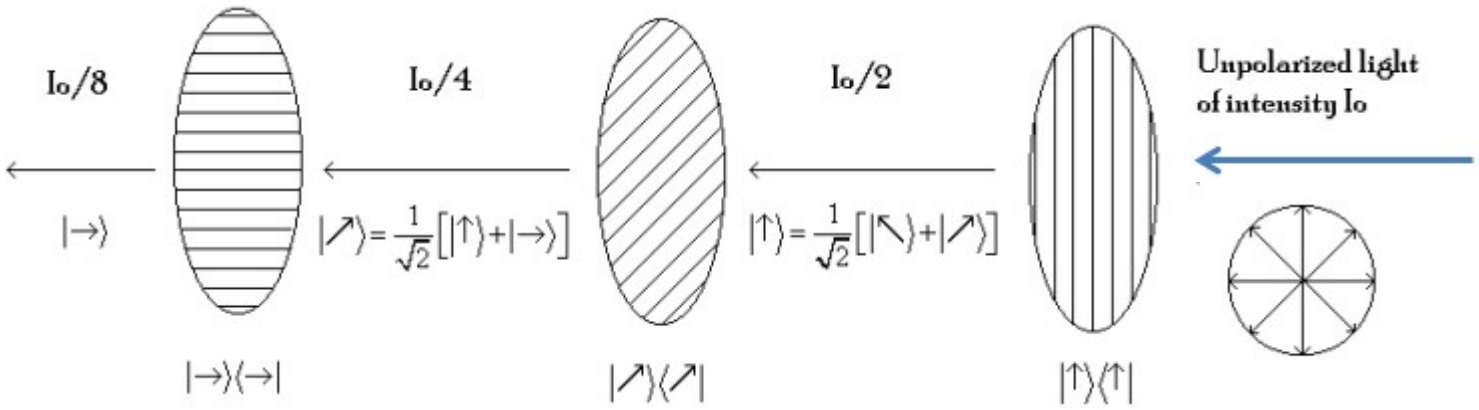
We've been forgetting about the third direction, S_y. There should be nothing special about the $\hat{x}$ direction versus $\hat{y}$, of course - and indeed if we run the experiment above using $\hat{y}$ instead of $\hat{x}$, we get the same results. But it seems like we've used up our mathematical freedom in defining the S_x states! Moreover, we know that S_x and S_y have to be distinct, since obviously we expect the same results yet again if we run the sequential S-G experiment in the $\hat{x}$ and $\hat{y}$ directions.

The only way out is to enlarge the space by allowing the vector components to be *complex*; then

See **Section on Bloch Sphere** for Explanation

$$S_y = \pm\hbar/2 \Rightarrow \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm i \end{pmatrix}.$$

VIII. Exploring the Three Polarizer "Paradox"

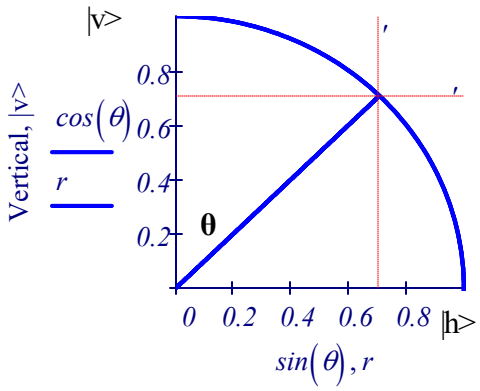


Quantum Mechanical Analysis (Refer to the Above Drawing)

A photon polarized at an **angle θ** with respect to the **Vertical** can be written as a **linear combination** (superposition) of a **vertically** polarized photon, |v>, and a **horizontally** polarized photon, |h>,. We say |v>, and |h>, are the polarization basis states, which means <v|v>, = <h|h> = 1 and <v|h> = <h|v> = 0.

$$|\Theta\rangle = |v\rangle\langle v|\Theta\rangle + |h\rangle\langle h|\Theta\rangle$$

Photon Polarization



Horizontal, |h>

From this figure we see that the projections of $|\Theta\rangle$ onto $|v\rangle$ ($\langle v|\Theta\rangle$) and $|h\rangle$ ($\langle h|\Theta\rangle$) are cos (Θ) and sin (Θ), respectively.

$$|\Theta\rangle = |v\rangle\cos(\Theta) + |h\rangle\sin(\Theta)$$

The probability that a photon polarized at an angle Θ will pass a vertical polarizer is

$$|\langle v|\Theta\rangle|^2 = \cos^2(\Theta)$$

The light incident on the first polarizer is unpolarized, but the photons that pass the vertical polarizer are vertically polarized. In other words **the photons are eigenfunctions of the measurement operato**r, which in this case is a vertically oriented linear polarizer. At this point only two experiments have definite outcomes.

1. The probability that vertically polarized photons will pass a second filter that is also vertically polarized is one. It is certain that a vertically polarized (Θ = 0) photon will pass a vertically polarized filter.

$$|\langle v|v\rangle|^2 = \cos^2(0^0) = 1$$

2. The probability that vertically polarized photons will pass a second filter that is horizontally polarized is zero. It is certain that a vertically polarized (Θ = π/2) photon will not pass a horizontally polarized filter.

$$|\langle h|v\rangle|^2 = \cos^2(90^0) = 0$$

For **<u>any other</u> orientation** of the second filter, quantum mechanics can only predict the probability that a **vertically polarized photon will pass**, and that probability is, of course,

$$|\langle \Theta \,|\, v\rangle|^2 = \cos^2(\Theta^0)$$

Now a vertically polarized photon may be written as a linear superposition of any other orthogonal basis states, for example $|45°\rangle$, and $|-45°\rangle$,.

$$|v\rangle = |45^0\rangle\langle 45^0|v\rangle + |-45^0\rangle\langle -45^0|v\rangle$$
$$|v\rangle = |45^0\rangle\cos(45^0) + |-45^0\rangle\cos(45^0$$
$$|v\rangle = |45^0\rangle.707 + |-45^0\rangle.707$$

If a 45° polarizer is inserted between the vertical and horizontal polarizers photons get through the horizontal polarizer that stopped them previously. Here is the quantum mechanical explanation. The probability $|\langle \Theta \,|\, v\rangle|^2$ that a vertically polarized photon will get through a polarizer oriented at an angle of 45° is, by above eqns, 1/2.

$$\left|\langle 45^0|v\rangle\right|^2 = \cos^2(45^0) = \frac{1}{2}$$

At this point the photon is in the state $|45°\rangle$, and according to the superposition principle a photon in this state can be written as a **linear combination of $|v\rangle$ and $|h\rangle$**,

$$|45^0\rangle = |v\rangle\langle v|45^0\rangle + |h\rangle\langle h|45^0\rangle$$
$$|45^0\rangle = |v\rangle\cos(45^0) + |h\rangle\sin(45^0$$

Therefore, the probability that this photon will pass the **<u>FINAL</u> horizontally (*h*) oriented** polarizer is

$$\left|\langle h|45^0\rangle\right|^2 = \sin^2(45^0) = \frac{1}{2} \qquad sin(45deg)^2 = 0.5$$

Alternatively, the probability that a photon emerging from the **vertical polarizer** will pass through the **<u>FINAL</u>** horizontal polarizer in the presence of an intermediate 45° polarizer can be calculated as follows:

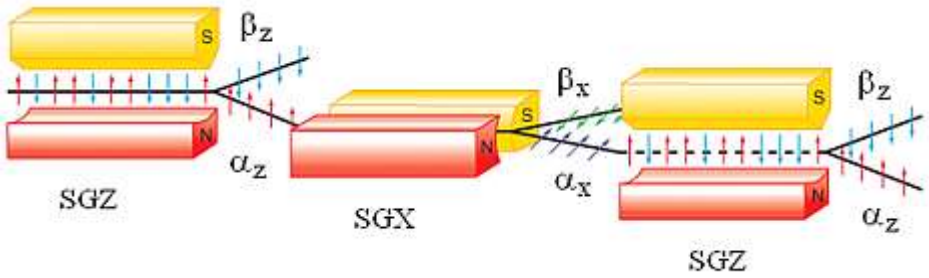
$$\left|\langle h|45^0\rangle\langle 45^0|v\rangle\right|^2 = \left|\sin(45^0)\cos(45^0)\right|^2 = \frac{1}{4} \qquad (sin(45deg)\cdot sin(45deg))^2 = 0.25$$

In other words, half of the photons that emerge from the vertical polarizer pass the 45° polarizer, and half of those pass the final horizontal polarizer. So 25% of the photons that pass the initial vertical polarizer also pass the final horizontal polarizer.

<u>The purpose of the following tutorial is to analyze the Stern-Gerlach experiment using matrix mechanics.</u>

Analysis of the Stern-Gerlach Experiment - Discovery of Electron Spin, 1922

Quantum Chemistry, Thomas Engel



Quantum Computing, Jozef Gruska

The quantum theory explanation is the following one: Passing an atom through a magnetic field amounts to a measurement of its magnetic alignment, and until you make such a measurement there is no sense in saying what the atom's magnetic alignment might be only when you make a measurement do you obtain one of only two possible outcomes, with equal probability, and those two possibilities are defined by the direction of the magnetic field that you use to make the measurement.

Actually, no matter how the magnetic field was lined up, it always splits the beam of atoms into two. (An exception to this is, as a result of interference, is shown on page 23.) As if each atom was forced somehow to take up either one or the other of just two possible orientations, dictated by the alignment of the magnets.

Silver atoms are deflected by an inhomogeneous magnetic field because of the two-valued magnetic moment associated with their unpaired 5s electron ($[Kr]5s^1 4d^{10}$). The beam of silver atoms entering the Stern-Gerlach magnet oriented in the z-direction (SGZ) on the left is unpolarized. This means it is a **mixture** of randomly spin-polarized Ag atoms. As such, it is **impossible to write a quantum mechanical wavefunctio**n for this initial state. It was only after modern quantum mechanics was founded, beginning in 1925, that physicists realized that the silver atom's magnetism is produced not by the orbit of its outermost electron but by that **electron's intrinsic spin**, which makes it act like a tiny bar magnet.

This situation is exactly analogous to the **Three-Polarizer "Paradox"** demonstration described in a previous section. Light emerging from an incandescent light bulb is unpolarized, a mixture of all possible polarization angles, so we can't write a wave function for it. The first Stern-Gerlach magnet plays the same role as the first polarizer, it forces the Ag atoms into one of measurement eigenstates - spin-up or spin-down in the z-direction. The only difference is that in the three-polarizer demonstration only one state was created - vertical polarization. Both demonstrations illustrate an important quantum mechanical postulate - the only values that are observed in a measurement are the eigenvalues of the measurement operator.

To continue with the analysis of the Stern-Gerlach demonstration we need vectors to represent the various spin states of the Ag atoms. We will restrict our attention to the x- and z- spin directions, although the spin states for the y-direction are also available.

Spin Eigenfunctions

Spin-up in the z-direction: $\alpha_z := \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ Spin-down in the z-direction: $\beta_z := \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

Spin-up in the x-direction: $\alpha_x := \frac{1}{\sqrt{2}} \cdot \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ Spin-down in the x-direction: $\beta_x := \frac{1}{\sqrt{2}} \cdot \begin{pmatrix} 1 \\ -1 \end{pmatrix}$

After the SGZ magnet, the spin-up beam (deflected toward the magnet's north pole) enters a magnet oriented in the x-direction, SGX. The α_z beam splits into α_x and β_x beams of equal intensity. This is because it is a **superposition of the x-direction spin eigenstate**s as shown below.

$$\frac{1}{\sqrt{2}}\cdot\left[\frac{1}{\sqrt{2}}\cdot\begin{pmatrix}1\\1\end{pmatrix}+\frac{1}{\sqrt{2}}\cdot\begin{pmatrix}1\\-1\end{pmatrix}\right]=\begin{pmatrix}1\\0\end{pmatrix}\qquad\frac{1}{\sqrt{2}}\cdot\left(\alpha_x+\beta_x\right)=\begin{pmatrix}1\\0\end{pmatrix}$$

Next the a_x beam is directed toward a second SGZ magnet and splits into two equal a_z and b_z beams. This happens because a_x is a superposition of the a_z and b_z spin states.

$$\frac{1}{\sqrt{2}}\cdot\left[\begin{pmatrix}1\\0\end{pmatrix}+\begin{pmatrix}0\\1\end{pmatrix}\right]=\begin{pmatrix}0.707\\0.707\end{pmatrix}\qquad\frac{1}{\sqrt{2}}\cdot\left(\alpha_z+\beta_z\right)=\begin{pmatrix}0.707\\0.707\end{pmatrix}$$

Operators (Pauli)

We can also **use the Pauli operators** (in units of h/4π) to analyze this experiment. The matrix operators associated with the two Stern-Gelach magnets are shown below.

SGZ operator: $SGZ:=\begin{pmatrix}1&0\\0&-1\end{pmatrix}$ SGX operator: $SGX:=\begin{pmatrix}0&1\\1&0\end{pmatrix}$

NOTE: SGY operator: $SGY:=\begin{pmatrix}0&-i\\i&0\end{pmatrix}$

The spin states **a_z and b_z** are **eigenfunction**s of the SGZ operator with **eigenvalues +1 and -1**, respectively:

$$SGZ\cdot\alpha_z=\alpha_z\quad SGZ\cdot\alpha_z=\begin{pmatrix}1\\0\end{pmatrix}\quad\alpha_z=\begin{pmatrix}1\\0\end{pmatrix}\qquad SGZ\cdot\beta_z=-\beta_z\quad SGZ\cdot\beta_z=\begin{pmatrix}0\\-1\end{pmatrix}\quad-\beta_z=\begin{pmatrix}0\\-1\end{pmatrix}$$

The spin states **a_x and b_x** are **eigenfunction**s of the SGX operator with **eigenvalues +1 and -1**, respectively:

$$SGX\cdot\alpha_x=\alpha_x\quad SGX\cdot\alpha_x=\begin{pmatrix}0.707\\0.707\end{pmatrix}\quad\alpha_x=\begin{pmatrix}0.707\\0.707\end{pmatrix}\quad SGX\cdot\beta_x=-\beta_x\quad SGX\cdot\beta_x=\begin{pmatrix}-0.707\\0.707\end{pmatrix}$$

The spin states a_x and b_x are **not eigenfunctions of the SGZ operator** as is shown below.

$$SGZ\cdot\alpha_x=\beta_x\qquad SGZ\cdot\alpha_x=\begin{pmatrix}0.707\\-0.707\end{pmatrix}\qquad SGZ\cdot\beta_x=\alpha_x\qquad SGZ\cdot\beta_x=\begin{pmatrix}0.707\\0.707\end{pmatrix}\qquad\beta_x=\begin{pmatrix}0.707\\-0.707\end{pmatrix}$$

And, of course, the spin states a_z and b_z are **not eigenfunctions** of the SGX operator as is shown below.

$$SGX\cdot\alpha_z=\beta_z\qquad SGX\cdot\alpha_z=\begin{pmatrix}0\\1\end{pmatrix}\qquad\alpha_z=\begin{pmatrix}1\\0\end{pmatrix}\qquad SGX\cdot\beta_z=\alpha_z\quad SGX\cdot\beta_z=\begin{pmatrix}1\\0\end{pmatrix}\qquad\beta_z=\begin{pmatrix}0\\1\end{pmatrix}$$

The Predicted Results After the SGX Magnet

The probability that an a_z Ag atom will emerge spin-up after passing through a SGX magnet:

Note: *The **arrow symbol** → below is used in Mathcad to evaluate an expression symbolically. Mathcad returns the result as another expression in terms of the variable and symbols in the original problem.*

$$\left|\langle \alpha_x | SGX | \alpha_z \rangle\right|^2 = ½ \qquad \left(\left|\alpha_x{}^T \cdot SGX \cdot \alpha_z\right|\right)^2 \rightarrow \frac{1}{2}$$

The probability that an a_z Ag atom will emerge spin-down after passing through a SGX magnet:

$$\left|\langle \beta_x | SGX | \alpha_z \rangle\right|^2 = ½ \qquad \left(\left|\beta_x{}^T \cdot SGX \cdot \alpha_z\right|\right)^2 \rightarrow \frac{1}{2}$$

The Predicted Results After the Final SGZ Magnet

The probability that an a_x Ag atom will emerge spin-up after passing through a SGZ magnet:

$$\left|\langle \alpha_z | SGZ | \alpha_x \rangle\right|^2 = ½ \qquad \left(\left|\alpha_z{}^T \cdot SGZ \cdot \alpha_x\right|\right)^2 \rightarrow \frac{1}{2}$$

The probability that an a_x Ag atom will emerge spin-down after passing through a SGZ magnet:

$$\left|\langle \beta_z | SGZ | \alpha_x \rangle\right|^2 = ½ \qquad \left(\left|\beta_z{}^T \cdot SGZ \cdot \alpha_x\right|\right)^2 \rightarrow \frac{1}{2}$$

The Predicted Results for the First SGZ Magnet

Now we deal with the most difficult part of the analysis. How does quantum mechanics predict what will happen when an unpolarized spin beam encounters the initial SGZ magnet. As mention earlier, an unpolarized spin beam is a **mixture** of all possible spin polarizations. We proceed by introducing the density operator, which is a more general quantum mechanical construct that can be used to represent both pure states and mixtures, as shown below.

$$\hat{\rho}_{pure} = |\Psi\rangle\langle\Psi| \qquad \hat{\rho}_{mixed} = \sum p_i |\Psi_i\rangle\langle\Psi_i|$$

In the equation on the right, p_i is the fraction of the mixture in the state Y_i. It is not difficult to elucidate the origin of the density operator and its utility in quantum mechanical calculations. The expectation value for a pure state Y for the measurement operator A is traditionally written as follows.

$$\langle A \rangle = \langle \Psi | \hat{A} | \Psi \rangle$$

Expansion of Y in the eigenfunctions of the measurement operator, followed by rearrangement of the brackets yields the calculation of the expectation value of A in terms of the product of density operator and the measurement operator, A.

$$\langle A \rangle = \langle \Psi | \hat{A} | \Psi \rangle = \sum_a \langle \Psi | \hat{A} | a \rangle \langle a | \Psi \rangle = \sum_a \langle a | \Psi \rangle \langle \Psi | \hat{A} | a \rangle = \sum_a \langle a | \hat{\rho} \hat{A} | a \rangle = Trace\left(\hat{\rho} \hat{A}\right)$$

We now show that the traditional method and the method using the trace function give the same result for the z-direction spin eigenfunctions.

$$\alpha_z^T \cdot SGZ \cdot \alpha_z = 1 \qquad tr\left(\alpha_z \cdot \alpha_z^T \cdot SGZ\right) = 1$$

$$\beta_z^T \cdot SGZ \cdot \beta_z = -1 \qquad tr\left(\beta_z \cdot \beta_z^T \cdot SGZ\right) = -1$$

An unpolarized beam can be written as a 50-50 mixture of any of the orthogonal spin eigenfunctions - α_z and β_z, or α_x and β_x, or α_y and β_y. Thus, according to the previous definition the density operator for an unpolarized spin beam is as follows.

$$\hat{\rho}_{mix} = \frac{1}{2}|\alpha_z\rangle\langle\alpha_z| + \frac{1}{2}|\beta_z\rangle\langle\beta_z| = \frac{1}{2}|\alpha_x\rangle\langle\alpha_x| + \frac{1}{2}|\beta_x\rangle\langle\beta_x| = \frac{1}{2}|\alpha_y\rangle\langle\alpha_y| + \frac{1}{2}|\beta_y\rangle\langle\beta_y|$$

Fifty percent of the silver atoms are deflected toward the north pole (a_z, eigenvalue +1) and fifty percent toward the south pole (b_z, eigenvalue -1). Therefore, the expectation value should be zero as is calculated below using both z- and x- spin directions.

$$tr\left[\left(\frac{1}{2}\cdot\alpha_z\cdot\alpha_z^T + \frac{1}{2}\cdot\beta_z\cdot\beta_z^T\right)\cdot SGZ\right] = 0 \qquad tr\left[\left(\frac{1}{2}\cdot\alpha_x\cdot\alpha_x^T + \frac{1}{2}\cdot\beta_x\cdot\beta_x^T\right)\cdot SGZ\right] = 0$$

An equivalent method of obtaining the same result is shown below.

$$\frac{1}{2}\cdot\alpha_z^T\cdot SGZ\cdot\alpha_z + \frac{1}{2}\cdot\beta_z^T\cdot SGZ\cdot\beta_z = 0 \qquad \frac{1}{2}\cdot\alpha_z^T\cdot SGZ\cdot\alpha_z + \frac{1}{2}\cdot\beta_z^T\cdot SGZ\cdot\beta_z = 0$$

IX. Entanglement

Two systems are in a special case of quantum mechanical superposition called entanglement if the measurement of one system is correlated with the state of the other system in a way that is stronger than correlations in the classical world. In other words, the states of the two systems are not separable.

To create entangled particles you essentially break a system into two, where the sum of the parts is known. For example, you can split a particle with spin of zero into two particles that necessarily will have opposite spins so that their sum is zero. We will explore the precise mathematical definitions of separability and entanglement later.

1.4.2 The physics path (To Quantum Entanglement)

The physics path is a pragmatic, measurement driven, avenue to quantum entanglement. It began with a paper by Dirac on **pair production** (Dirac 1930) and some sixteen years later was followed by a transparent and profound statement by John Wheeler that captures the very essence of quantum entanglement: 'if one of these photons is linearly polarized in one plane, then the photon that **goes off in the opposite direction with equal momentum** is **linearly polarized** in the perpendicular plane ' (Wheeler 1946-). Wheeler made his statement in reference to a positron–electron annihilation process, $e^+e^- \rightarrow \gamma_1\gamma_2$, that leads to the emission of two quanta in opposite directions. Ward followed with a disclosure of the derivation of the quantum entanglement probability amplitude

$$|\psi\rangle = (|x_1, y_2\rangle - |y_1, x_2\rangle)$$

Mathematically, this means Entanglement is a Sum of Products of Wave-functions.

It should be noted that this probability amplitude is essential for the correct derivation of the final quantum probability for the quantum scattering equation published by Pryce and Ward (1947).
It should also be stated categorically that the above $|\psi\rangle$ expression for the probability amplitude includes and contains all the physics relevant to quantum entanglement experiments. All this physics was done pre-Bell theorem in a complete vacuum of philosophical discussions and in the total absence of concern, or preoccupation, with hidden variable theories.
What should be kept in mind is that even though today all of the developments in the field of quantum entanglement revolve around the probability amplitude for quantum entanglement $|\psi\rangle = (|x_1, y_2\rangle - |y_1, x_2\rangle)$ there is almost no acknowledgement of its origin or the physics path that led to its discovery. This monograph is designed to provide a perspective on quantum entanglement from the philosophical and the physics perspectives by including all the relevant literature. This approach removes the 'cloud of mystery' that surround quantum entanglement.

1.5 The field of quantum entanglement

The emergence of the combined words quantum entanglement, in the open literature, appears to go back to the mid-late 1980s (Ghirardi et al 1987). This was a few years after the optical experiments on quantum entanglement by Aspect et al (1981, 1982a,1982b).
Today the fireld of quantum entanglement is enormous and it is divided roughly into three main sub fields: quantum cryptography, quantum teleportation, and quantum computing. Quantum communications is part of quantum cryptography. On paper, judging by citations, these sub fields have been heavily influenced by the ideas and concepts derived from the philosophical path to quantum entanglement. On the other hand, also judging from citations, the acknowledgement of the physics path has been utterly minuscule. This almost non-existing recognition has persisted albeit the all-important probability amplitude for quantum entanglement, which was discovered in a vacuum of philosophical arguments:

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|x\rangle_1|y\rangle_2 - |y\rangle_1|x\rangle_2)$$

See Bell States - 2nd Page Down

was reintroduced into the mainstream literature of quantum entanglement with the following alternative formulations.

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|+\rangle_1|-\rangle_2 - |-\rangle_1|+\rangle_2) \qquad |\psi\rangle = \frac{1}{\sqrt{2}}(|+-\rangle - |-+\rangle) \qquad |\psi\rangle = |+1\rangle|-1\rangle + |-1\rangle|+1\rangle$$

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle) \qquad |\psi\rangle = \frac{1}{\sqrt{2}}(|1\rangle|0\rangle - |0\rangle|1\rangle) \qquad |\psi\rangle = \frac{1}{\sqrt{2}}(|10\rangle - |01\rangle)$$

Entanglement is locally created. $|\psi\rangle = (|\psi_1\rangle \otimes |\psi_2\rangle)/\sqrt{2}$

Like tearing a photograph in two and sending it to two different locations. They are nonlocally correlated, but correlation was locally created. But it is a correlation that is stronger than for non-quantum particles. But it is just a property of how quantum states combine.

Entanglement

Tutorial: *Overview On quantum entanglement*, J. Ladvánszky, Ericsson Hungary

Quantum entanglement is a physical phenomenon which occurs when pairs or groups of particles are generated, interact, or share physical proximity in ways such that the **quantum state of each particle cannot be described independently of the state of the other(s)**, even when the particles are separated by a large distance—instead, a quantum state must be described for the system as a whole. Measurements of physical properties such as position, momentum, spin, and polarization, performed on entangled particles are found to be correlated. For example, if a pair of particles is generated in such a way that their total spin is known to be zero, and one particle is found to have clockwise spin on a certain axis, the spin of the other particle, measured on the same axis, will be found to be counterclockwise, as is to be expected due to their entanglement.

An entangled system is defined to be **one whose quantum state cannot be factored as a product of states of its local constituents**; that is to say, they are not individual particles but are an inseparable whole. In entanglement, **one constituent cannot be fully described without considering the other(s)**. Note that the state of a composite system is always expressible as a sum, or superposition, of products of states of local constituents; it is entangled if this sum necessarily has more than one term.

Just as classical bits are the fundamental building block of classical computers, quantum bits--or "qubits"--are the basic unit of information in quantum computers. Whereas classical bits can either have a value of 0 or 1, qubits can be in a combination of the states |0> and |1>. If the qubit is **not exactly in the state |0> or in the state |1>,** but rather in **some combination of both** the |0> and |1> states, then we say the qubit is in a "superposition" of the two states. The paradox is that a measurement made on either of the particles apparently collapses the state of the entire entangled system—and does so instantaneously.

Quantum mechanical framework

Consider **two noninteracting systems A and B,** with respective Hilbert spaces H_A and H_B. The Hilbert space of the composite system is the tensor product

$$H_A \otimes H_B$$

If the first system is in state $|\psi\rangle_A$ and the second in state $|\psi\rangle_B$, the state of the composite system is $|\psi\rangle_A \otimes |\phi\rangle_B$.

Not all states are separable states (and thus product states). Fix a basis for H_A and a basis $|\psi\rangle_A$ for H_B. The most general state in $H_A \otimes H_B$ is of the form $|\psi\rangle_{AB} = \sum_{i,j} c_{ij}|i\rangle_A \otimes |j\rangle_B$

This state is separable if there exist vectors $[c_i^A],[c_j^B]$ so that $c_{ij}=c_i^A c_j^B$, yielding $|\psi\rangle_A=\sum_i c_i^A|i\rangle_A$ and $|\phi\rangle_B=\sum_j c_j^B|j\rangle_B$.

It is inseparable if for any vectors $[c_i^A],[c_j^B]$ at least for one pair of coordinates c_i^A, c_j^B we have $c_{ij}\neq c_i^A c_j^B$.

If a state is inseparable, it is called an entangled state.

For example, given two basis vectors $\{|0\rangle_A,|1\rangle_A\}$ of H_A and two basis vectors $\{|0\rangle_B,|1\rangle_B\}$ of H_B, the following is an entangled state: $\frac{1}{\sqrt{2}}(|0\rangle_A \otimes |1\rangle_B - |1\rangle_A \otimes |0\rangle_B)$

If the composite system is in this state, it is **impossible** to attribute to either system A or system B **a definite pure state**. Another way to say this is that while the von Neumann entropy of the whole state is zero (as it is for any pure state), the entropy of the subsystems is greater than zero. In this sense, the systems are "entangled". This has specific empirical ramifications for interferometry. It is worthwhile to note that the above example is one of four Bell states, which are (maximally) entangled pure states (pure states of the $H_A \otimes H_B$ space, but which cannot be separated into pure states of each H_A and H_B).

Measurement:

When we measure a qubit that is **exactly in the |0> state or |1> state**, then the qubit **will remain in that state.** However, if we measure a qubit that is in a **superposition**, then this **superposition collapses** from being in a combination of two states to being exactly in one of the two states. We cannot predict if the superposition will collapse into either the |0> or the |1> state with certainty, but we **can only know the probabilities** of being measured in either of the two states.

Entanglement:

It turns out that quantum states can extend over multiple qubits. When two or more qubits are entangled, measuring one of the qubits has an effect on the probability distributions of collapse for the other qubits. A Bell pair is a special 2-qubit quantum state, with properties that make it especially useful for certain applications.

Two indistinguishable particles with spin 1/2

LibreTexts Physics, Graeme Ackland, U of Edinburgh

If we have two identical fermions of spin 1/2, confined in the same region, what is the appropriate wavefunction? In the scattering case we could measure spins far from the interaction, and if we knew that the total spins is conserved, spins can be associated with each particle. In the bound state we cannot tell which particle we are measuring, so the ket must contain both spin and spatial wavefunctions of both particles.

Assuming the spins do not interact, we can separate the two-particle spin wavefunction into $\sigma(1,2)=\sigma_1\sigma_2$. We also know the appropriate one particle basis states $\uparrow 1, \downarrow 1, \uparrow 2, \downarrow 2$, where $\uparrow 1$ represents "particle 1" in spinor state $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$. The combinations for indistinguishable particles are then:

$$\uparrow_1\uparrow_2, \quad \downarrow_1\downarrow_2, \quad (\uparrow_1\downarrow_2 + \downarrow_1\uparrow_2)/\sqrt{2}, \quad (\uparrow_1\downarrow_2 - \downarrow_1\uparrow_2)/\sqrt{2}$$

Operating on these with $\hat{P}_{12}$ yields eigenvalues 1, 1, 1 and -1 respectively. $\mathbf{S}^2$=S(S+1) yields 2, 2, 2 and 0, S_z yields 1, -1, 0 and 0. Thus the demands of indistinguishability couples the spins of two identical particles into a triplet (S=1) and a singlet (S=0). The spin-1 vector has three possible M_s component values - hence the triplet.

What are the Bell states?

The term Bell pairs actually describes one of four entangled two qubit quantum states, known collectively as the four "Bell states." Two of the Bell states give an equal superposition such that both of the qubits end up in the same state when measured, with a 50% chance that both will be in either the |0> or |1> state. The other two Bell pairs give an equal superposition such that both of the qubits end in opposite states when measured. This means that if the first qubit is measured in |0>, then the second qubit will be measured in |1> and vice versa.

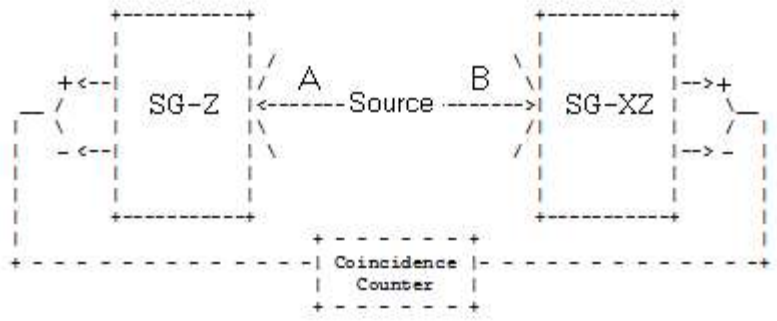
Definition of Entanglement (Bell States)

Bell Pair Symbol	Mathematical Representation	
|Φ+>	(|00> + |11>)/ √2	Same States
|Φ->	(|00> - |11>)/√2	
|Ψ+>	(|01> + |10>)/√2	Opposite States
|Ψ->	(|01> - |10>)/√2	

In each of the Bell pairs, if one of the two qubits is measured, then we know exactly what the other qubit will be when it is measured. Let's consider one of |Φ+> or |Φ->. These are the two Bell pairs where both of the qubits must end up in the **same state** when measured. If we measure the first qubit in the state |0>, we know that the second qubit must be in |0> when we measure it. Even if these two qubits were on opposite ends of the globe and we measured them immediately one after another, if we found |0> |0> for the first qubit, then the second qubit would have to also be in the |0> |0> state. **Entanglement is necessary for a wide range of quantum networking protocols**, and Bell pairs are the most widely used entangled states for these protocols.

Quantum Correlations Simplified

In order to explore the conflict between quantum mechanics and local realism a spin-1/2 pair is prepared in an **entangled singlet state** and the individual particles travel in opposite directions on the y-axis to a pair of Stern-Gerlach detectors which are set up to measure spin in the x-z plane. Particle A's spin is measured along the z-axis, and particle B's spin is measured at any angle θ with respect to the z-axis. The experimental setup is shown below.



The entangled singlet spin state is written in both the z- and θ-direction spin eigenstates.

$$|\Psi\rangle = \frac{1}{\sqrt{2}}\left[|\uparrow\rangle_A|\downarrow\rangle_B - |\downarrow\rangle_A|\uparrow\rangle_B\right] = \frac{1}{\sqrt{2}}\left[\begin{pmatrix}\cos(\frac{\theta}{2})\\ \sin(\frac{\theta}{2})\end{pmatrix}_A \otimes \begin{pmatrix}-\sin(\frac{\theta}{2})\\ \cos(\frac{\theta}{2})\end{pmatrix}_B - \begin{pmatrix}-\sin(\frac{\theta}{2})\\ \cos(\frac{\theta}{2})\end{pmatrix}_A \otimes \begin{pmatrix}\cos(\frac{\theta}{2})\\ \sin(\frac{\theta}{2})\end{pmatrix}_B\right] = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\-1\\0\end{pmatrix}$$

Spin-up
Eigenvalue +1 $\varphi_u(\theta) := \begin{pmatrix}\cos\left(\frac{\theta}{2}\right)\\ \sin\left(\frac{\theta}{2}\right)\end{pmatrix}$

Spin-down
Eigenvalue -1 $\varphi_d(\theta) := \begin{pmatrix}-\sin\left(\frac{\theta}{2}\right)\\ \cos\left(\frac{\theta}{2}\right)\end{pmatrix}$

If particle A is observed to be spin-up in the z-direction (eigenvalue +1), particle B is spin-down in the z-direction due to the singlet nature of the entangled state.

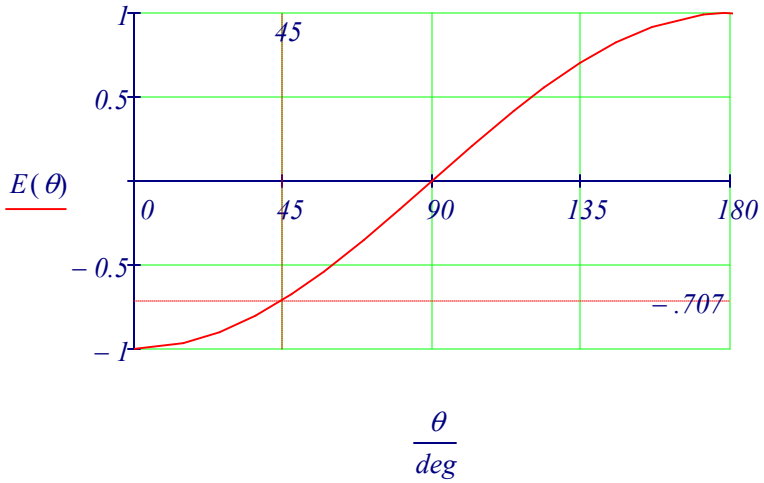
Probability B will be found on measurement to be spin-up in the θ-direction yielding a **composite eigenvalue** of **+1** is: $\left(\varphi_u(\theta)^T \cdot \varphi_d(0)\right)^2 \text{ simplify } \rightarrow \frac{1}{2} - \frac{\cos(\theta)}{2}$

Probability B will be found on measurement to be spin-down in the θ-direction yielding a composite eigenvalue of **-1** is: $\left(\varphi_d(\theta)^T \cdot \varphi_d(0)\right)^2 \text{ simplify } \rightarrow \frac{\cos(\theta)}{2} + \frac{1}{2}$

Therefore the overall quantum correlation or expectation value is:

$$E(\theta) := \left(\varphi_u(\theta)^T \cdot \varphi_d(0)\right)^2 - \left(\varphi_d(\theta)^T \cdot \varphi_d(0)\right)^2 \text{ simplify } \rightarrow -\cos(\theta)$$

The expectation value as a function of the measurement angle difference is displayed below. In what follows we will concentrate on the data for only 0 degrees and 45 degrees, and show that a local realistic model is consistent with the 0-degree result but not the 45-degree result.



If the observers measure their spins in the same direction (both θ = 0 deg or both θ = 45 deg) quantum mechanics predicts they will get opposite values due to the singlet nature of the spin state. In other words, the combined expectation value is -1 for these measurements as shown in the figure above. However, if they measure their spins at 0 and 45 degrees, the expectation value is -0.707.

Realists believe that objects have well-defined properties prior to and independent of observation. Specific 0- and 45-deg spin states are assigned to the particles in the first two columns, with each particle in one of four equally probable spin orientations consistent with the composite singlet state. The next two columns show that these assignments agree with the quantum predictions when both spins are measured at the same angle. The last column shows that these spin assignments disagree with the quantum prediction when one spin is measured at 0 degrees and the other at 45 degrees.

Particle A	Particle B	$\hat{S}_0(A)\cdot\hat{S}_0(B)$	$\hat{S}_{45}(A)\cdot\hat{S}_{45}(B)$	$\hat{S}_0(A)\cdot\hat{S}_{45}(B)$
$\lvert\uparrow\rangle\lvert\square\rangle$	$\lvert\downarrow\rangle\lvert\square\rangle$	−1	−1	−1
$\lvert\uparrow\rangle\lvert\square\rangle$	$\lvert\downarrow\rangle\lvert\square\rangle$	−1	−1	1
$\lvert\downarrow\rangle\lvert\square\rangle$	$\lvert\uparrow\rangle\lvert\square\rangle$	−1	−1	1
$\lvert\downarrow\rangle\lvert\square\rangle$	$\lvert\uparrow\rangle\lvert\square\rangle$	−1	−1	−1
Realist	Value	−1	−1	0
Quantum	Value	−1	−1	−0.707

This brief analysis demonstrates that there are conceptually simple, Stern-Gerlach like, experiments on spin-1/2 systems which can adjudicate the conflict between local realism and quantum mechanics.

In addition to the disagreement shown in the last column of the table, quantum theory asserts that the realist's spin states are invalid. The spin operator at an angel θ to the vertical in the xz-plane is

$$Op(\theta) := \varphi_u(\theta)\cdot\varphi_u(\theta)^T - \varphi_d(\theta)\cdot\varphi_d(\theta)^T \ simplify \rightarrow \begin{pmatrix} cos(\theta) & sin(\theta) \\ sin(\theta) & -cos(\theta) \end{pmatrix}$$

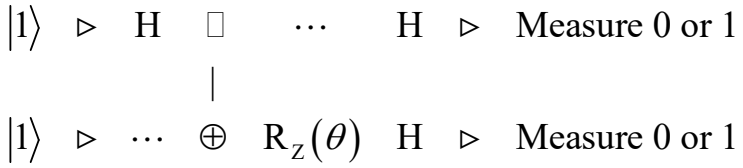
The operators for spin measurements at 0 and 45 degrees in the xz-plane do not commute.

$$Op(0\cdot deg)\cdot Op(45\cdot deg) - Op(45\cdot deg)\cdot Op(0\cdot deg) = \begin{pmatrix} 0 & 1.414 \\ -1.414 & 0 \end{pmatrix}$$

Therefore, according to quantum theory a particle's spin cannot be simultaneously well-defined for both 0 and 45 degrees.

Addendum

According to Richard Feynman it takes a quantum computer to simulate quantum pheonomenon. The following quantum circuit produces results that are in agreement with experiment as summarized in the graph above. The Hadamard and CNOT gates create the singlet state from the |11> input. $R_Z(\theta)$ is the rotation of the measuring device of the second spin. The final Hadamard gates prepare the system for measurement in the x-basis. See arXiv:1712.05642v2 for further detail.



The quantum operators redquired to execute this circuit are:

$$I := \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad H := \frac{1}{\sqrt{2}}\cdot\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \qquad R_z(\theta) := \begin{pmatrix} 1 & 0 \\ 0 & e^{i\cdot\theta} \end{pmatrix} \qquad CNOT := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

$$BellCircuit(\theta) := kronecker(H, H)\cdot kronecker\left(I, R_z(\theta)\right)\cdot CNOT\cdot kronecker(H, I)$$

The circuit is run for $\theta = \pi/4$ to demonstrate that it produces the result highlighted in the graph above. In addition, by varying θ it can be shown that the circuit reproduces the entire plot of $E(\theta)$. There are four output states shown below. If the spins are measured in the same state, |00> or |11>, the eigenvalue is +1, if they are different, |01> or |10>, the eigenvalue is -1. The probability for each output state is calculated on the right.

Output state	Eigenvalue	Probability
$\lvert 00\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$	1	$\left[\left\lvert \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}^T \cdot BellCircuit\left(\frac{\pi}{4}\right)\cdot \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \right\rvert\right]^2 = 0.0732$
$\lvert 01\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$	-1	$\left[\left\lvert \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}^T \cdot BellCircuit\left(\frac{\pi}{4}\right)\cdot \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \right\rvert\right]^2 = 0.4268$

Output state	Eigenvalue	Probability
$\|10\rangle = \begin{pmatrix}0\\1\end{pmatrix} \otimes \begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix}0\\0\\1\\0\end{pmatrix}$	-1	$\left[\left\| \begin{pmatrix}0\\0\\1\\0\end{pmatrix}^T \cdot BellCircuit\left(\frac{\pi}{4}\right) \cdot \begin{pmatrix}0\\0\\0\\1\end{pmatrix} \right\|\right]^2 = 0.4268$
$\|11\rangle = \begin{pmatrix}0\\1\end{pmatrix} \otimes \begin{pmatrix}0\\1\end{pmatrix} = \begin{pmatrix}0\\0\\0\\1\end{pmatrix}$	1	$\left[\left\| \begin{pmatrix}0\\0\\0\\1\end{pmatrix}^T \cdot BellCircuit\left(\frac{\pi}{4}\right) \cdot \begin{pmatrix}0\\0\\0\\1\end{pmatrix} \right\|\right]^2 = 0.0732$

Expectation value or correlation coeficient: $0.0732 - 0.4268 - 0.4268 + 0.0732 = -0.707$

A classical computer manipulates bits which are in well-defined states consisting of 0s and 1s.This entangled two-spin experiment demonstrates that simulation of quantum physics requires a computer that can manipulate 0s and 1s, superpositions of 0 and 1, and entangled superpositions of 0s and 1s. Simulation of quantum physics requires a quantum computer, and the circuit shown above is a quantum computer.

An alternative computational method using projection operators:

Output state	Eigenvalue	Probability
$\|00\rangle = \begin{pmatrix}1\\0\end{pmatrix} \otimes \begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix}1\\0\\0\\0\end{pmatrix}$	1	$\left[\left\| kronecker\left[\begin{pmatrix}1&0\\0&0\end{pmatrix}, \begin{pmatrix}1&0\\0&0\end{pmatrix}\right] \cdot BellCircuit\left(\frac{\pi}{4}\right) \cdot \begin{pmatrix}0\\0\\0\\1\end{pmatrix} \right\|\right]^2 = 0.0732$
$\|01\rangle = \begin{pmatrix}1\\0\end{pmatrix} \otimes \begin{pmatrix}0\\1\end{pmatrix} = \begin{pmatrix}0\\1\\0\\0\end{pmatrix}$	-1	$\left[\left\| kronecker\left[\begin{pmatrix}1&0\\0&0\end{pmatrix}, \begin{pmatrix}0&0\\0&1\end{pmatrix}\right] \cdot BellCircuit\left(\frac{\pi}{4}\right) \cdot \begin{pmatrix}0\\0\\0\\1\end{pmatrix} \right\|\right]^2 = 0.4268$

Output state	Eigenvalue	Probability
$\lvert 10\rangle = \begin{pmatrix}0\\1\end{pmatrix} \otimes \begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix}0\\0\\1\\0\end{pmatrix}$	-1	$\left[\left\lvert kronecker\left[\begin{pmatrix}0&0\\0&1\end{pmatrix},\begin{pmatrix}1&0\\0&0\end{pmatrix}\right]\cdot BellCircuit\left(\frac{\pi}{4}\right)\cdot\begin{pmatrix}0\\0\\0\\1\end{pmatrix}\right\rvert\right]^2 = 0.4268$
$\lvert 11\rangle = \begin{pmatrix}0\\1\end{pmatrix} \otimes \begin{pmatrix}0\\1\end{pmatrix} = \begin{pmatrix}0\\0\\0\\1\end{pmatrix}$	1	$\left[\left\lvert kronecker\left[\begin{pmatrix}0&0\\0&1\end{pmatrix},\begin{pmatrix}0&0\\0&1\end{pmatrix}\right]\cdot BellCircuit\left(\frac{\pi}{4}\right)\cdot\begin{pmatrix}0\\0\\0\\1\end{pmatrix}\right\rvert\right]^2 = 0.0732$

Measuring only one spin using a projection operator and the identity:

$$\left[\left\lvert kronecker\left[\begin{pmatrix}1&0\\0&0\end{pmatrix},\begin{pmatrix}1&0\\0&1\end{pmatrix}\right]\cdot BellCircuit\left(\frac{\pi}{4}\right)\cdot\begin{pmatrix}0\\0\\0\\1\end{pmatrix}\right\rvert\right]^2 = 0.5$$

$$\left[\left\lvert kronecker\left[\begin{pmatrix}1&0\\0&1\end{pmatrix},\begin{pmatrix}1&0\\0&0\end{pmatrix}\right]\cdot BellCircuit\left(\frac{\pi}{4}\right)\cdot\begin{pmatrix}0\\0\\0\\1\end{pmatrix}\right\rvert\right]^2 = 0.5$$

$$\left[\left\lvert kronecker\left[\begin{pmatrix}0&0\\0&1\end{pmatrix},\begin{pmatrix}1&0\\0&1\end{pmatrix}\right]\cdot BellCircuit\left(\frac{\pi}{4}\right)\cdot\begin{pmatrix}0\\0\\0\\1\end{pmatrix}\right\rvert\right]^2 = 0.5$$

$$\left[\left\lvert kronecker\left[\begin{pmatrix}1&0\\0&1\end{pmatrix},\begin{pmatrix}0&0\\0&1\end{pmatrix}\right]\cdot BellCircuit\left(\frac{\pi}{4}\right)\cdot\begin{pmatrix}0\\0\\0\\1\end{pmatrix}\right\rvert\right]^2 = 0.5$$

X. Q Operators, Gates, Algorithms, Polarization: Query Models - Oracles

Tutorial: Quantum Computing, An Applied Approach, Jack Hidary

The earliest quantum algorithms are known as "**black box" or "query model" quantum algorithms**. Black boxes are theoretical constructs; they may or may not have an efficient implementation. For this reason, they are often called **oracles**. In these cases, there is an **underlying function which is unknown to us.** However, we are able to construct another function, called an oracle, which we can **query to determine the relationship of specific inputs with specific outputs.** More specifically, we can query the oracle function with specific inputs in the quantum register and reversibly write the output of the oracle function into that register. That is, we have access to an oracle O_f such that

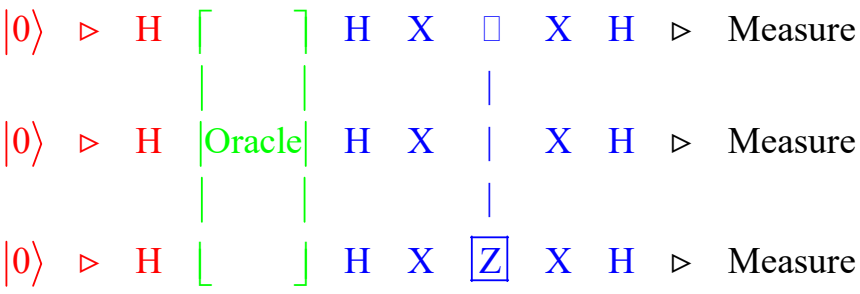
$$O_f|x\rangle = |x \oplus f(x)\rangle$$

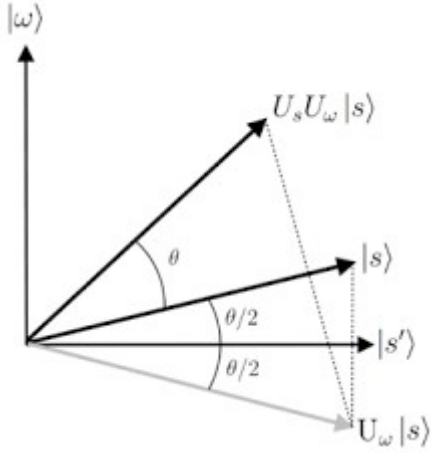
where $\oplus$ denotes addition modulo-2. .This can seem like "cheating" at first — how could we construct a circuit to perform O_f? And how could we know it's an efficient circuit? One reason to think about quantum algorithms in the query model is because it **provides a lower bound on the number of steps (gates)**. Each query is *at least* one step in the algorithm, so if it cannot be done efficiently with queries, it can certainly not be done efficiently with gates. Thus, the query model can be useful for ruling out fast quantum algorithms.

However, the query model can also be used to prove fast quantum algorithms relative to the oracle. We can give both a quantum computer and a classical computer access to the same oracle and see which performs better. It's possible to prove lower bounds or exact expressions for the number of queries in the classical and quantum cases, thereby making it possible to prove computational advantages relative to oracles. Examples of quantum algorithms with provable relativized speedups include Deutsch's algorithm and the Berstein-Vazirani algorithm.

These black box/oracle algorithms are one particular class of quantum algorithms. There are other algorithm classes such as quantum simulation.

Example: Grover's Quantum Search Algorithm (See Section XVII)





Grover's algorithm relies on an oracle. An oracle can be viewed as a black box that performs an operation on a quantum state that is not readily specified by universal quantum gates. In Grover's algorithm, an oracle is implemented such that it flips the sign of |x> iff x is a state we are looking for (the 'correct' quantum state). This can be expressed as

$$|x\rangle \xrightarrow{\mathcal{O}} (-1)^{f(x)}|x\rangle$$

with $f(x) = 1$ if x is the correct state and $f(x) = 0$ otherwise. We assume that a function f is given as a black box, or oracle, means that it is not possible to obtain knowledge about f by any other means than by evaluating it on points of its domain.

Methodology for Grover's Search Algorithm

Mathematically, one can think of the algorithm as inverting a function

$f(x) : \{0, 1, 2 \cdots n\} \rightarrow \{0, 1\}$, where $f(x) = 0$, $x \neq a$; $f(x) = 1$, $x = a$, and the goal is to find a.

Exploring Unary Quantum Operators - Gates

We will examine the set of **one-qubit**, or unary, quantum operators. The first three operators we will examine are the **Pauli matrices, X Y Z**. These three matrices along with the identity matrix and all of their ±1 and ±i multiples constitute what is known as the Pauli group. **A unary operator is a gate** that takes **single input bit**, and a **binary** operator is one that takes **two input bits**. For example, it is a linear transformation of the **Hamiltonian Operator, *H***, that maps normalized (unit) vectors to other normalized vectors. Since H is 2-dimensional, a unary quantum operator can be represented by a 2 × 2 matrix.

X Operator: which is the NOT operator. It is denoted by the symbol ⊕. It is also denoted by the Pauli Matrix, σ_x,

Y Operator, also denoted σ_y, which **rotates the state vector about the y axis**.

Z Operator, also denoted σ_z, which **rotates the state vector about the z axis** (also called the **phase flip operator** since it flips it by π radians or 180 degrees) (also known as the bit flip operator and can be referred to as x)

R(φ) General phase shift operator. When we apply this operator we leave the **state |0> as is** and we take the state |1> and rotate it by the angle (or phase) denoted by φ, as specified in the matrix

$$R_1(\varphi) := \begin{pmatrix} 1 & 0 \\ 0 & e^{-\varphi} \end{pmatrix}$$

S Operator, additional phase shift operators that are special cases of the Rφ matrix where φ = π/2. The S operator thus rotates the state **about the z-axis by 90°**.

T Operator which rotates the state **about the z-axis by 45°**. If we give φ the value of π=4. Note: $S = T^2$

H, Hadamard Operator: --> qubit in **superposition state** where probability of measuring 0 = probability measuring 1.

Pauli Spin Matrices, X, Y, Z $(\sigma_x, \sigma_y, \sigma_z)$ **Note:** Matrices X and Y on this page have Mathcad names of X_{dot} and Y_{dot}

$$X := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad Y := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad Z := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad R(\varphi) := \begin{pmatrix} 1 & 0 \\ 0 & e^{-\varphi} \end{pmatrix} \quad T := \begin{pmatrix} 1 & 0 \\ 0 & e^{i\frac{\pi}{4}} \end{pmatrix}$$

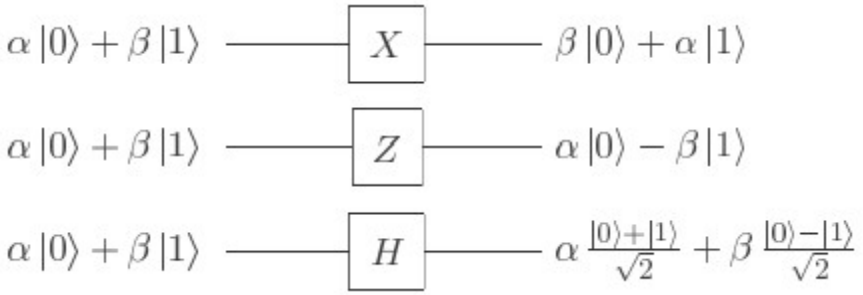
$$S := \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} \quad I := \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad P(\varphi) := \begin{pmatrix} 1 & 0 \\ 0 & e^{\varphi} \end{pmatrix}$$

$$U(\theta, \phi, \lambda) := \begin{bmatrix} \cos\left(\frac{\theta}{2}\right) & -e^{i\cdot\lambda}\cdot\sin\left(\frac{\theta}{2}\right) \\ e^{i\cdot\phi}\cdot\sin\left(\frac{\theta}{2}\right) & e^{i\cdot(\phi+\lambda)}\cdot\cos\left(\frac{\theta}{2}\right) \end{bmatrix}$$

$$L0 := \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad H\cdot L0 = \begin{pmatrix} 0.707 \\ 0.707 \end{pmatrix}$$

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}\cdot\begin{pmatrix} e \\ f \end{pmatrix} \rightarrow \begin{pmatrix} a\cdot e + b\cdot f \\ c\cdot e + d\cdot f \end{pmatrix}$$

$$U\left(\frac{\pi}{2}, 0, \pi\right) = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\cdot\frac{1}{\sqrt{2}}$$



Gate Identities

Quantum Computing: An Applied Approach, Jack Hidary

$$HXH = Z \qquad HZH = X \qquad HYH = -Y \qquad H^{\dagger} = H = H^{-1}$$

$$X^2 = Y^2 = Z^2 = I \qquad H = (X + Z)/\sqrt{2} \qquad H^2 = I \qquad SWAP_{12} = C_{12}C_{21}C_{12}$$

$$X \cdot Z = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \qquad Z \cdot X = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

$$X := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad Y := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad Z := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad H := \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

$$H \cdot Z \cdot H = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad -H \cdot Y \cdot H = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad H \cdot X \cdot H = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad H = \begin{pmatrix} 0.707 & 0.707 \\ 0.707 & -0.707 \end{pmatrix}$$

$$H = \begin{pmatrix} 0.707 & 0.707 \\ 0.707 & -0.707 \end{pmatrix} \qquad H^T = \begin{pmatrix} 0.707 & 0.707 \\ 0.707 & -0.707 \end{pmatrix} \qquad H^{-1} = \begin{pmatrix} 0.707 & 0.707 \\ 0.707 & -0.707 \end{pmatrix}$$

$$I := \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad X^2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad Y^2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad Z^2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad H^2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\frac{1}{\sqrt{2}} \cdot (X + Z) = \begin{pmatrix} 0.707 & 0.707 \\ 0.707 & -0.707 \end{pmatrix} \qquad H = \begin{pmatrix} 0.707 & 0.707 \\ 0.707 & -0.707 \end{pmatrix}$$

$$S := \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} \qquad P(\varphi) := \begin{pmatrix} 1 & 0 \\ 0 & e^{\varphi} \end{pmatrix} \qquad R(\varphi) := \begin{pmatrix} 1 & 0 \\ 0 & e^{-\varphi} \end{pmatrix} \qquad T := \begin{pmatrix} 1 & 0 \\ 0 & e^{i\frac{\pi}{4}} \end{pmatrix}$$

$$CNOT := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \qquad C := CNOT \qquad SWAP := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Gates, States, and Circuits, Gavin Crooks

$$kronecker(X, X) = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \qquad kronecker(Y, Y) = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix} \qquad kronecker(Z, Z) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Bloch Rotation Decomposition

Decompositions of 1-qubit gates into single rotations about a particular axis

$$R_{\vec{n}}(\theta) = e^{-i\frac{1}{2}\theta(n_x X + n_y Y + n_z Z)}$$

$$R_{\vec{n}}(\theta) = \begin{bmatrix} \cos(\frac{1}{2}\theta) - i n_z \sin(\frac{1}{2}\theta) & -n_y \sin(\frac{1}{2}\theta) - i n_x \sin(\frac{1}{2}\theta) \\ n_y \sin(\frac{1}{2}\theta) - i n_x \sin(\frac{1}{2}\theta) & \cos(\frac{1}{2}\theta) + i n_z \sin(\frac{1}{2}\theta) \end{bmatrix}$$

$$R_x(\theta) = R_{\vec{n}}(\theta), \quad \vec{n} = (1, 0, 0)$$
$$R_y(\theta) = R_{\vec{n}}(\theta), \quad \vec{n} = (0, 1, 0)$$
$$R_z(\theta) = R_{\vec{n}}(\theta), \quad \vec{n} = (0, 0, 1)$$

Cofactor, CoF, of a Matrix

Complementary Minor of a Square Matrix

The complementary minor of a matrix A is the matrix $A^{(ij)}$ whose entries $C_{i,j}$ are (n -1) x (n -1) submatrices of A formed by removing the i^{th} row and j^{th} column of A.

Cofactor of a Square Matrix

The cofactor matrix of a matrix A is the matrix C whose entries $C_{i,j}$ are the determinants of the (n -1) x (n -1) submatrices of A formed by removing the i^{th} row and j^{th} column of A. We call $C_{i,j}$ the i, j^{th} cofactor of A, CoF(A, i, j).

Change the Starting Index (ORIGIN) of Arrays from 0 to 1

$ORIGIN := 1$

Function RR: Remove Row R from Matrix M

$$RR(M,R) := \begin{| RR \leftarrow rows(M) \\ CC \leftarrow cols(M) \\ SM \leftarrow M_{RR-1,CC} \\ \text{for } i \in 1..RR \\ \quad \text{for } j \in 1..CC \\ \quad\quad SM_{i,j} \leftarrow M_{i,j} \text{ if } i < R \\ \quad\quad SM_{i-1,j} \leftarrow M_{i,j} \text{ if } i > R \\ RemR \leftarrow SM$$

Function RC: Remove Column C from Matrix M

$$RC(M,C) := \begin{| RR \leftarrow rows(M) \\ CC \leftarrow cols(M) \\ SM \leftarrow M_{RR,CC-1} \\ \text{for } i \in 1..RR \\ \quad \text{for } j \in 1..CC \\ \quad\quad SM_{i,j} \leftarrow M_{i,j} \text{ if } j < C \\ \quad\quad SM_{i,j-1} \leftarrow M_{i,j} \text{ if } j > C \\ RemC \leftarrow SM$$

Verify CoFactor Program, CoF

$$A := \begin{pmatrix} 2 & 5 & -1 \\ 0 & 3 & 4 \\ 1 & -2 & -5 \end{pmatrix}$$

CoF(A,3,2) = -8

$CoF(A,3,2) = -8$

Calculate CoFactor, CoF, of Matrix M, Row R, Column C

$$CoF(M,R,C) := \begin{| SM \leftarrow RC(M,C) \\ SM \leftarrow RR(SM,R) \\ sign \leftarrow (-1)^{(R+C)} \\ Cof \leftarrow sign \cdot |SM|$$

CoFactor Gate Identities

$$SWAP_{12} = C_{12}C_{21}C_{12} \qquad CoF(SWAP,1,2) = 0 \qquad CoF(C,1,2)\cdot CoF(C,2,1)\cdot CoF(C,1,2) = 0$$

$$C_{12}X_1C_{12} = X_1X_2$$
$$C_{12}Y_1C_{12} = Y_1X_2$$
$$C_{12}Z_1C_{12} = Z_1$$
$$C_{12}X_2C_{12} = X_2$$
$$C_{12}Y_2C_{12} = Z_1Y_2$$
$$C_{12}Z_2C_{12} = Z_1Z_2$$
$$R_{z,1}(\theta)C_{12} = C_{12}R_{z,1}(\theta)$$
$$R_{x,2}(\theta)C_{12} = C_{12}R_{x,2}(\theta)$$

$ORIGIN := 0$

Exploring - Unary Operators/Functions/Quantum Gates

Quantum Computing: An Applied Approach, Jack Hidary, Second Edition , pg. 28 - 33

$Zero := \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ $One := \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

NOT: $X \cdot Zero = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ $X \cdot One = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

Y Op: $Y \cdot Zero = \begin{pmatrix} 0 \\ i \end{pmatrix}$ $Y \cdot One = \begin{pmatrix} -i \\ 0 \end{pmatrix}$

Z Op: $Z \cdot Zero = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ $Z \cdot One = \begin{pmatrix} 0 \\ -1 \end{pmatrix}$

S Op: $S \cdot Zero = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ $S \cdot One = \begin{pmatrix} 0 \\ i \end{pmatrix}$

Identity: $I \cdot Zero = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ $I \cdot One = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

T Op: $T \cdot Zero = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ $T \cdot One = \begin{pmatrix} 0 \\ 0.707 + 0.707i \end{pmatrix}$

H Op: $H \cdot Zero = \begin{pmatrix} 0.707 \\ 0.707 \end{pmatrix}$ $H \cdot One = \begin{pmatrix} 0.707 \\ -0.707 \end{pmatrix}$

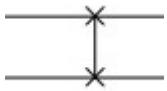
Phase: $R_1(30deg) \cdot Zero = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ $R_1(30deg) \cdot One = \begin{pmatrix} 0 \\ 0.592 \end{pmatrix}$

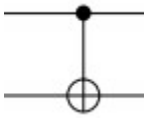
XZ Op: $Z \cdot (X \cdot Zero) = \begin{pmatrix} 0 \\ -1 \end{pmatrix}$ $Z \cdot (X \cdot One) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

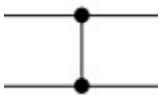
Exploring - Binary Operators/Functions/Quantum Gates/Circuit Models

$OO := \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$ $O1 := \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$ $SWAP := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$ $CNOT := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ $CZ := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$

Quantum Circuit Diagrams ==>







Explorations of Operators

$'10 := \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$ $'11 := \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$ $SWAP \cdot O1 = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$ $CNOT \cdot '10 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$ $CZ \cdot '10 = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$ $CZ \cdot '11 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ -1 \end{pmatrix}$

The **CNOT gate** copies the bit x if y = 0 and gives -x if y = 1, and is the reversible equivalent of the COPY operation. It is reversible because there is a one-to-one correspondence between the initial state & final state. The CNOT operation is a simple permutation of the basis vectors. It can be shown that using single-bit gates $x \to 1 \oplus x$ or $x \to \neg x$ and the CNOT gate, it is possible to construct only linear functions if we limit ourselves to classical operations.

Ternary Operators: Toffoli and Fredkin Operators - Math

We have discussed both unary and binary operators. Now let's consider the ternary or 3-qubit operators. First, we have the **Toffoli operator**, also known as the **CCNOT gate**. Just as in the CNOT operator, we have control and target qubits. In this case, the first two qubits are control and the third is the target qubit. Both control qubits have to be in state |1> for us to modify the target qubit. Another way of thinking about this is that the first two qubits (x and y) have to satisfy the Boolean AND function — if that equals TRUE then we apply NOT to the target qubit, z. We can represent this action as ,

The nonlinearity of the gate is $(x, y, z) \mapsto (x, y, (z \oplus xy))$ he Toffoli gate performs the NAND operation reversibly. The Toffoil gate can be used to reproduce reversibly all the classical logic circuits. It is a universal gate for all reversible operations of Boolean logic.

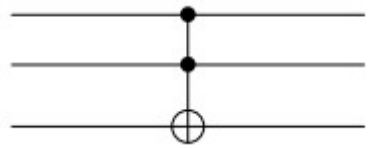
Or as a matrix, CCNOT

$$CCNOT := \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

As an example, we apply this gate to the state |110>, 110

$$'110 := \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \qquad CCNOT \cdot '110 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

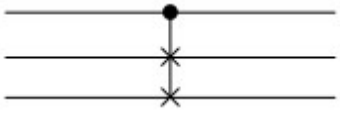
In circuit diagrams, we use the following to denote the Toffoli Gate



Next, let's consider **the Fredkin gate**, also known as the **CSWAP gate**. When we apply this operator, the first qubit is the control and the other two are the target qubits. If the first qubit is in state |0> we do nothing and if it is in state |1> then we SWAP the other two qubits with each other. The matrix representing this operations is

$$CSWAP := \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \qquad CSWAP \cdot '110 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

In circuit diagrams we use this symbol for the Fredkin operator



XI. The Bloch Sphere: Is a physical representation of all possible qubit states.

Each qubit is in its essence a vector on Bloch's sphere.

The Three ZXY Axes: State: |0> Z (Up), State: (|+>) X Front (+), State: (|i>) Y Side (i)

0 State (Z Up)	1 State (Z Down)	+ State (X Front)	- State (X Back)	i State (Y Right)	-i State (Y Left)
$Z_u := \begin{pmatrix} 1 \\ 0 \end{pmatrix}$	$Z_d := \begin{pmatrix} 0 \\ 1 \end{pmatrix}$	$X_f := \frac{1}{\sqrt{2}} \cdot \begin{pmatrix} 1 \\ 1 \end{pmatrix}$	$X_b := \frac{1}{\sqrt{2}} \cdot \begin{pmatrix} 1 \\ -1 \end{pmatrix}$	$Y_r := \frac{1}{\sqrt{2}} \cdot \begin{pmatrix} 1 \\ i \end{pmatrix}$	$Y_l := \frac{1}{\sqrt{2}} \cdot \begin{pmatrix} 1 \\ -i \end{pmatrix}$

Create a Bloch Sphere (XYZ) With Angles: θ, ϕ to Represent Any Qubit State

NOTE: Index i is an i_{dot}

X,Y,Z are Xdot dot, Ydot dot' Z dot dot

$$n := 50 \qquad i := 0..n \qquad j := 0..n \qquad \theta_i := \pi \cdot \frac{i}{n} \qquad \phi_j := 2\pi \cdot \frac{j}{n}$$

$$X_{i,j} := \sin(\theta_i) \cdot \cos(\phi_j) \qquad Y_{i,j} := \sin(\theta_i) \cdot \sin(\phi_j) \qquad Z_{i,j} := \cos(\theta_i)$$

Next, the coordinates of a quantum qubit are calculated and displayed on the Bloch sphere as a white dot. As the polar and azimuthal angles are changed, you will need to rotate the figure to see where the white dot is on the surface of the Bloch sphere.

Note: The reason the angle θ is given as θ/2 is to setup angle between orthogonal basis |0> and |1> so that cos(π/2) = 0, i.e. Prob'ity = 0.

We can represent any state by the angles θ, ϕ, and γ

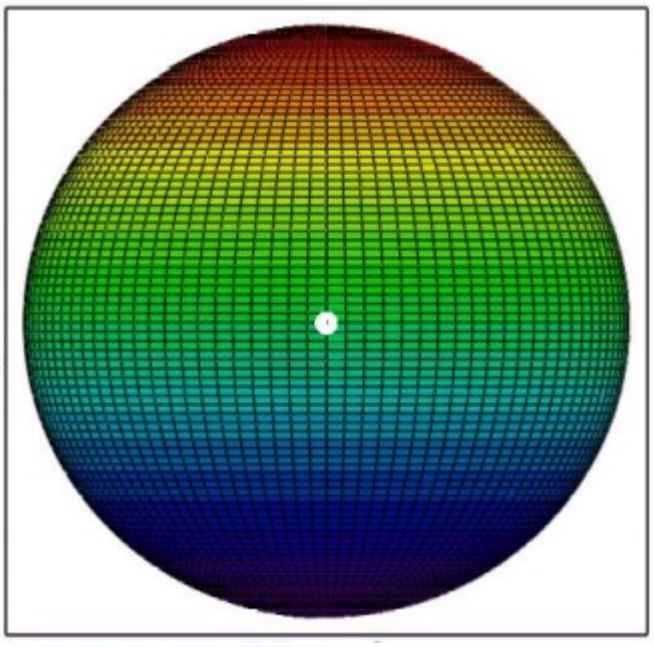
$$|\psi\rangle = e^{i\gamma}\left(\cos\frac{\theta}{2}|0\rangle + e^{i\varphi}\sin\frac{\theta}{2}|1\rangle\right)$$

$$\theta 1 := \frac{\pi}{2} \qquad \phi 1 := 0$$

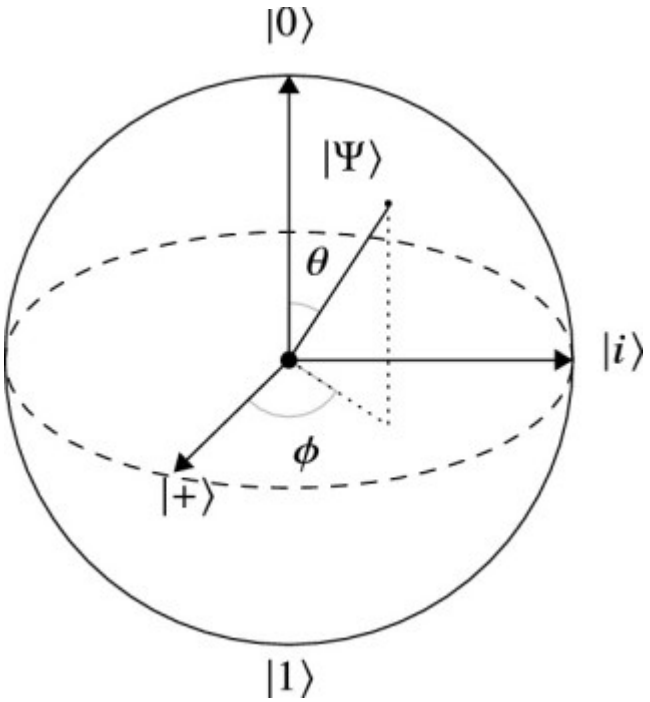
$$\Psi(\theta 1, \phi 1) := \cos\left(\frac{\theta 1}{2}\right) \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \exp(\phi 1) \cdot \sin\left(\frac{\theta 1}{2}\right) \cdot \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\Psi(\theta 1, \phi 1) = \begin{pmatrix} 0.707 \\ 0.707 \end{pmatrix}$$

$$XX_{i,j} := \sin(\theta 1) \cdot \cos(\phi 1) \qquad ZZ_{i,j} := \cos(\theta 1) \qquad YY_{i,j} := \sin(\theta 1) \cdot \sin(\phi 1)$$



$(X, Y, Z), (XX, YY, ZZ)$



The Bloch Sphere - Continued

The Bloch sphere is a nice way to visualize quantum states and to identify orthogonal states. Furthermore, because diametrically opposite states in the Bloch sphere are orthogonal it also gives insight in which particular states are orthogonal. However, it is only possible to do this for single qubit states. When multiple qubit states are considered, t is not possible to visualize states in such a way

Dirac Notation for Bloch Sphere Equatorial +, −, i+, and i−

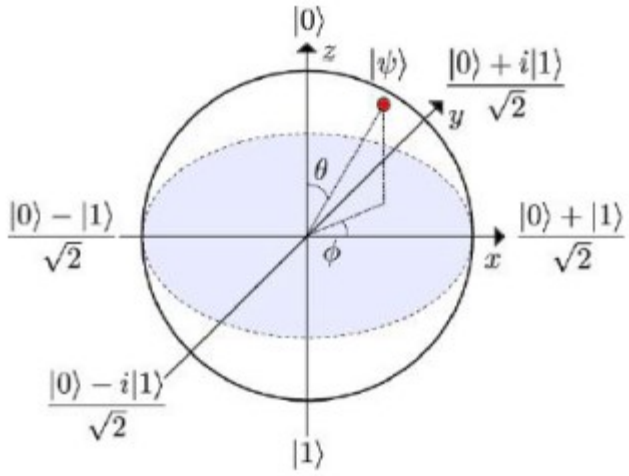
These |+> and |−> states differ by a minus sign on the |1> state. More formally, we call this difference a relative phase. The term phase has numerous meanings in physics - in this context, it refers to an angle. The minus sign is related to the angle π (180°) by Euler's identity: $e^{i\pi} = -1$.

$$|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \qquad |i+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + i|1\rangle)$$

$$|-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) \qquad |i-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - i|1\rangle)$$

Note: This View Flips the "0" |0> |1> Orientation to "1" |1> |0> Orientation

The θ and the ϕ angles are not equivalent in the Bloch sphere. First, they have **different ranges** -- one is π and the other is 2π. More importantly, ϕ is a rotation around a fixed axis, while θ is a rotation around a non-fixed axis that is moving with ϕ. **For ϕ=0 this axis is y**, for ϕ=π/2 it is x, and for every other ϕ it is everything in between in the x−y plane.



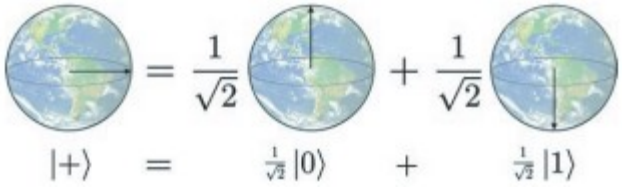
As we can see in above figure, one of the advantages of visualization with the Bloch sphere is that we can **represent superposition states** such as

$$\frac{|0\rangle + |1\rangle}{\sqrt{2}}$$

as we see at the X axis. We can also **differentiate** between states that contain **different phases** as is shown in the states along the **X and Y** axes. Let us return to computational universality which we treated above. Now that we have introduced the Bloch sphere, another way to think about a set of gates that satisfies universal computation is one which enables us to reach any point on the Bloch sphere.

See: Quantum Computing: An Applied Approach, Hidary

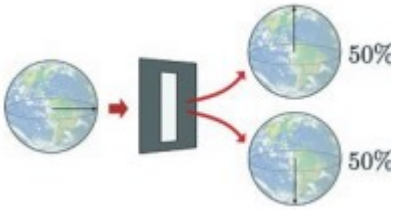
A perfect superposition of |0⟩ and |1⟩
corresponds to the quantum state |+⟩
and points, figuratively speaking,
towards the equator (x-axis) of the sphere.



$$|\uparrow_x\rangle = a|\uparrow_z\rangle + b|\downarrow_z\rangle = \begin{pmatrix} a \\ b \end{pmatrix}$$

$$\frac{|0\rangle + |1\rangle}{\sqrt{2}}$$

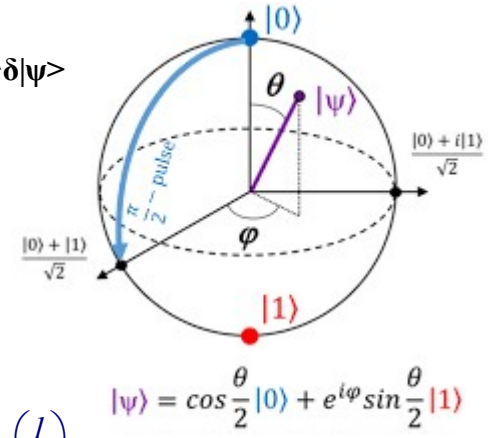
Measuring the "equator" state |+⟩
along the north-south axis results in
"north" or "south" with equal probability.



The Basic Building Blocks of Quantum Computing,
Ellerhoff

Expressions for the Bloch Vector Probabilities: Symbol for Bloch Sphere Vector ^n

Let ^n be a Bloch Sphere Basis Vector: $\hat{n} = (\langle\psi|\delta_x|\psi\rangle, \langle\psi|\delta_y|\psi\rangle, \langle\psi|\delta_z|\psi\rangle) = \langle\psi|\hat{\delta}|\psi\rangle$



Expectation Value: Complex Conjugate

$$\langle\psi|\delta_x|\psi\rangle = \left(\cos\left(\frac{\theta}{2}\right) \quad e^{-i\cdot\phi}\cdot\sin\left(\frac{\theta}{2}\right)\right)\cdot\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\cdot\begin{pmatrix}\cos\left(\frac{\theta}{2}\right)\\ e^{i\cdot\phi}\cdot\sin\left(\frac{\theta}{2}\right)\end{pmatrix}$$

Simplify the Above Expression:

The Square X Matrix Flips the Sign --> $X = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$ ----> $\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\cdot\begin{pmatrix}0\\ 1\end{pmatrix} \rightarrow \begin{pmatrix}1\\ 0\end{pmatrix}$

Note: X, θ, ϕ are X_{dot}, θ_{dot}, ϕ_{dot}

Simplify Expression →

$$\left(\cos\left(\frac{\theta}{2}\right) \quad e^{-i\cdot\phi}\cdot\sin\left(\frac{\theta}{2}\right)\right)\cdot\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\cdot\begin{pmatrix}\cos\left(\frac{\theta}{2}\right)\\ e^{i\cdot\phi}\cdot\sin\left(\frac{\theta}{2}\right)\end{pmatrix} \rightarrow \cos\left(\frac{\theta}{2}\right)\cdot\sin\left(\frac{\theta}{2}\right)\cdot e^{-\phi\cdot i} + \cos\left(\frac{\theta}{2}\right)\cdot\sin\left(\frac{\theta}{2}\right)\cdot e^{\phi\cdot i}$$

Simplifies To → $\left(e^{\phi\cdot i} + e^{-i\cdot\phi}\right)\cdot\left(\cos\left(\frac{\theta}{2}\right)\cdot\sin\left(\frac{\theta}{2}\right)\right) = 2\cos(\phi)\cdot\left(\cos\left(\frac{\theta}{2}\right)\cdot\sin\left(\frac{\theta}{2}\right)\right) = \sin(\theta)\cdot\cos(\phi)$

Similarly:

$n_x = \sin(\theta)\cdot\cos(\phi)$ $\quad n_y = \sin(\theta)\cdot\sin(\phi)$ $\quad n_z = \cos(\phi)$

$\langle\psi|\delta_x|\psi\rangle = \sin(\theta)\cdot\cos(\phi)$

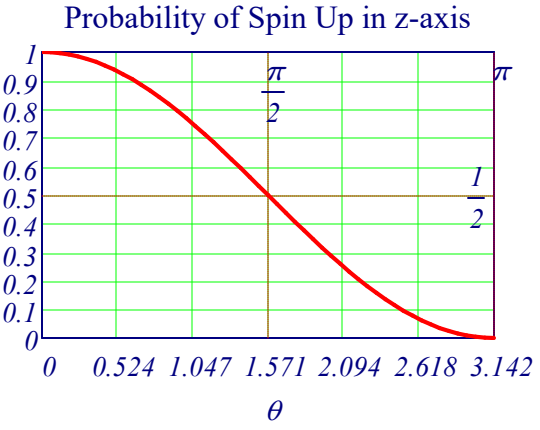
Thus All States |ψ⟩ can be expressed by some Bloch basis vector ^n, |ψ⟩ = |↑n⟩

Probability of spin up in z-axis is: $|\langle\uparrow_z|\uparrow_n\rangle|^2 = \cos^2(\theta/2) = 1/2(1+\cos(\theta))$

$|\langle\uparrow_z|\uparrow_n\rangle|^2 = 1/2(1 + \hat{n} * \hat{m})$

1 if ^n*^m = 1
1/2 if ^n*^m = 0
0 if ^n*^m = -1

$\frac{1}{2}\cdot(1+\cos(\theta))$



The Bloch Sphere - Continued

Tutorial: A Course in Quantum Computing, Michael Loceff

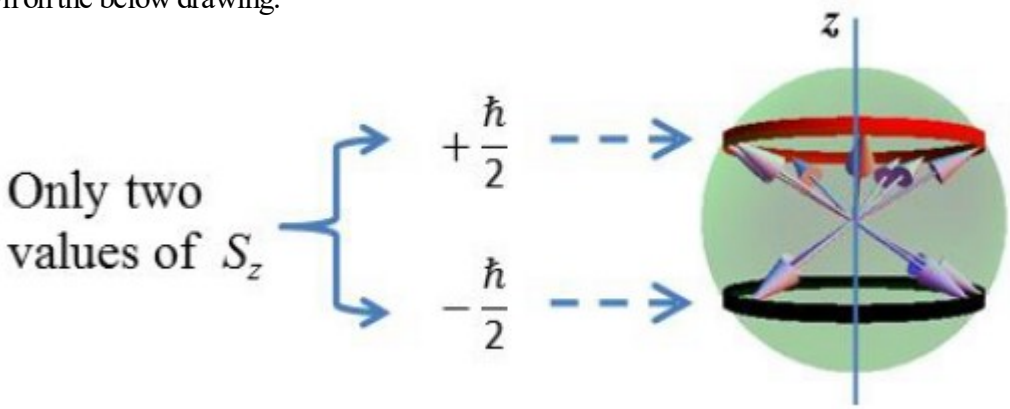
Spin is a property that every electron possesses. Some properties like charge and mass are the same for all electrons, while others like position and momentum vary depending on the electron in question and the exact moment at which we measure. The spin, or more accurate term spin state of an electron has aspects of both. There is an overall magnitude associated with an electron's spin state that does not change. It is represented by the number 1/2, a value shared by all electrons at all times. But then each election can have its own unique vector orientation that varies from electron-to-electron or moment-to-moment.

Spin has a 3-D direction and a scalar magnitude and we can break it into the two aspects, its scalar magnitude,

$$S = |S| = \sqrt{S_x^{\,2} + S_y^{\,2} + S_z^{\,2}}$$

and a unit vector that embodies only its orientation (direction) $\dfrac{S}{|S|}$

S, the spin magnitude, is the same for all electrons under all conditions. Its value is $\frac{\sqrt{3}}{2}\hbar$ where ħ is a tiny number known as Plank's constant.
But, actual measurements of spin along the z-axis only give values of $S_z = \left(+\frac{\hbar}{2}\right)$ or $\left(-\frac{\hbar}{2}\right)$
The situation is shown on the below drawing.



$0.577 \cdot \sqrt{\frac{3}{2}} = 0.707$

Why there is electron's projection onto the z-axis is not the entire length of the vector, that is, either straight up at (+√3/2) ħ or straight down at (−√3/2) ħ. The electron stubbornly wants to give us only a fraction of that amount, ≈ 57.7%. This corresponds to two groups. The "up group" which forms the angle θ ≈ 55°.

This smaller value is due to the Heisenberg Uncertainty Principle. If the spin were to collapse to a state that was any closer to the vertical ±z-axis, we would have too much simultaneous knowledge about its x- and y-components (too close to (0) and its z-component (too close to (±√3/2) ħ. This would violate the Heisenberg Uncertainty Principle, which requires the combined variation of these observables be larger than a fixed constant. Therefore, S_z must give up some of its claim on the full spin magnitude, $\left(\frac{\sqrt{3}}{2}\right)\hbar$

|+i> and |-i> States. We give a name to the state of the electrons in the (+) group: we call it the $|+\rangle_z$ state (or simply the |+⟩ state, since we consider the z-axis to be the preferred axis in which to project the spin).
We say that the (-) group is in the $|-\rangle_z$ (or just the |-⟩ state. Verbally, these two states are pronounced "plus ket" and "minus ket.

The Bell states are maximally entangled superpositions of two-particle states. Consider two spin-1/2 particles created in the same event. **There are four maximally entangled wave functions** representing their collective spin states. Each particle has two possible spin orientations and therefore the composite state is represented by a 4-vector in a four-dimensional Hilbert space.

$$|\Phi_p\rangle = \frac{1}{\sqrt{2}}[|\uparrow_1\rangle|\uparrow_2\rangle + |\downarrow_1\rangle|\downarrow_2\rangle] = \frac{1}{\sqrt{2}}\left[\begin{pmatrix}1\\0\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix} + \begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}0\\1\end{pmatrix}\right] = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\0\\1\end{pmatrix} \qquad \Phi_p = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\0\\1\end{pmatrix}$$

$$|\Phi_m\rangle = \frac{1}{\sqrt{2}}[|\uparrow_1\rangle|\uparrow_2\rangle - |\downarrow_1\rangle|\downarrow_2\rangle] = \frac{1}{\sqrt{2}}\left[\begin{pmatrix}1\\0\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix} - \begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}0\\1\end{pmatrix}\right] = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\0\\-1\end{pmatrix} \qquad \Phi_p = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\0\\-1\end{pmatrix}$$

$$|\Psi_p\rangle = \frac{1}{\sqrt{2}}[|\uparrow_1\rangle|\downarrow_2\rangle + |\downarrow_1\rangle|\uparrow_2\rangle] = \frac{1}{\sqrt{2}}\left[\begin{pmatrix}1\\0\end{pmatrix}\otimes\begin{pmatrix}0\\1\end{pmatrix} + \begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix}\right] = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\1\\0\end{pmatrix} \qquad \Phi_p = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\1\\0\end{pmatrix}$$

$$|\Psi_m\rangle = \frac{1}{\sqrt{2}}[|\uparrow_1\rangle|\downarrow_2\rangle - |\downarrow_1\rangle|\uparrow_2\rangle] = \frac{1}{\sqrt{2}}\left[\begin{pmatrix}1\\0\end{pmatrix}\otimes\begin{pmatrix}0\\1\end{pmatrix} - \begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix}\right] = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\-1\\0\end{pmatrix} \qquad \Phi_p = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\-1\\0\end{pmatrix}$$

The wave functions are not separable and consequently the entangled particles represented by these wave functions **do not have separate identities or individual properties**, they behave like a **single entity**. Individually the spins don't have a definite polarization, yet there is a definite spin orientation relationship between them. For example, if the spin orientation of particle 1 is learned through measurement, the spin orientation of particle 2 is also immediately known no matter how far away it may be. (The Appendix shows how such measurements destroy entanglement, forcing both particles into well-defined spin states.) Entanglement implies nonlocal phenomena which in the words of Nick Herbert are "unmediated, unmitigated and immediate." The Bell states can be generated from two classical bits with the use of a quantum circuit involving a **Hadamard (H) gate, the identity (I) and a controlled-not gate (CNOT)** as shown in Section IV and below . The H gate operates on the top bit creating a superposition which controls the operation of the CNOT gate. The classical state on the left also serves as an index for the Bell state created from it: 0, 1, 2, 3.

kronecker(M, N) Multiplies matrix N by each element of matrix M, returning an M•N by M•N array. Arguments: M and N are square matrices.

Bell State Generator, BSG

$$BSG := CNOT \cdot kronecker(H, I)$$

The controlled-NOT gate, CNOT, acts on a pair of qubits, with one acting as 'control' and the other as 'target'. It performs a **NOT** on the target, **if and only if, the control bit is |1>**. If the control qubit is in a superposition, this gate creates entanglement.

$$OO = \begin{pmatrix}1\\0\\0\\0\end{pmatrix} \qquad '10 = \begin{pmatrix}0\\0\\1\\0\end{pmatrix} \qquad O1 = \begin{pmatrix}0\\1\\0\\0\end{pmatrix} \qquad '11 = \begin{pmatrix}0\\0\\0\\1\end{pmatrix}$$

$$BSG \cdot OO = \begin{pmatrix}0.707\\0\\0\\0.707\end{pmatrix} \qquad BSG \cdot '10 = \begin{pmatrix}0.707\\0\\0\\-0.707\end{pmatrix} \qquad BSG \cdot O1 = \begin{pmatrix}0\\0.707\\0.707\\0\end{pmatrix} \qquad BSG \cdot '11 = \begin{pmatrix}0\\0.707\\-0.707\\0\end{pmatrix}$$

Xii. Simulating Spin Operators and Spin Space

LibreTexts: *Introductory Quantum Mechanics - Spin Operators*

The basic principles of quantum theory can be demonstrated very simply by exploring the properties of electron spin using Heisenberg's formulation of quantum mechanics which is usually referred to as matrix mechanics. The matrix formulation provides clear illustrations of the following essential quantum mechanical concepts: eigenvector, operator, eigenvalue, expectation value, the linear superposition, and the commutation relations.

Four quantum numbers are required to describe an electron in quantum mechanics. The last of these is the spin quantum number, s. The electron has a spin component in the x-, y-, and z-directions and for each of these directions the electron can have a value of ↑ spin-up or ↓ spin-down, or +1 and -1 in units of h/4π. These six spin states are represented by vectors as is shown below.

XY Z Axes Spin States (Up and Down) and Operators: Math

Transpose of Complex Conjugate (Shift")^T

$$S_{xu} := \frac{1}{\sqrt{2}}\cdot\begin{pmatrix}1\\1\end{pmatrix} \qquad S_{xd} := \frac{1}{\sqrt{2}}\cdot\begin{pmatrix}1\\-1\end{pmatrix} \qquad \left(\overline{S_{xu}}\right)^T = (0.707 \quad 0.707) \qquad \left(\overline{S_{xd}}\right)^T = (0.707 \quad -0.707)$$

$$S_{yu} := \frac{1}{\sqrt{2}}\cdot\begin{pmatrix}1\\i\end{pmatrix} \qquad S_{yd} := \frac{1}{\sqrt{2}}\cdot\begin{pmatrix}1\\-i\end{pmatrix} \qquad \left(\overline{S_{yu}}\right)^T = (0.707 \quad -0.707i) \qquad \left(\overline{S_{yd}}\right)^T = (0.707 \quad 0.707i)$$

$$S_{zu} := \begin{pmatrix}1\\0\end{pmatrix} \qquad S_{zd} := \begin{pmatrix}0\\1\end{pmatrix} \qquad \left(\overline{S_{zu}}\right)^T = (1 \quad 0) \qquad \left(\overline{S_{zd}}\right)^T = (0 \quad 1)$$

Let's look at the the **y-direction spin states because they are complex**, and therefore are slightly more difficult to deal with. In Dirac notation these four bra and ket Y vectors are written as $|S_{yu}\rangle$, $|S_{yd}\rangle$, $\langle S_{yu}|$, and $\langle S_{yd}|$. Note that the **bra-vectors are the transpose of the complex conjugate of the ket-vectors**. It is also easy to show that these spin vectors in the x-, y-, and z-directions form orthonormal basis sets. That means they are normalized and orthogonal to each other.

$$\left(\overline{S_{xu}}\right)^T\cdot S_{xu} = 1 \qquad \left(\overline{S_{xd}}\right)^T\cdot S_{xd} = 1 \qquad \left(\overline{S_{xu}}\right)^T\cdot S_{xd} = 0$$

$$\left(\overline{S_{yu}}\right)^T\cdot S_{yu} = 1 \qquad \left(\overline{S_{yd}}\right)^T\cdot S_{yd} = 1 \qquad \left(\overline{S_{yu}}\right)^T\cdot S_{yd} = 0$$

$$\left(\overline{S_{zu}}\right)^T\cdot S_{zu} = 1 \qquad \left(\overline{S_{zd}}\right)^T\cdot S_{zd} = 1 \qquad \left(\overline{S_{zu}}\right)^T\cdot S_{zd} = 0$$

In Dirac notation we would write the first row as: $\langle S_{xu}|S_{xu}\rangle = \langle S_{xd}|S_{xd}\rangle = 1$, $\langle S_{xu}|S_{xd}\rangle = 0$. In other words the **projection of the spin states onto themselves is 1** (normalized) and the projection onto the other state is zero (orthogonal). Momentum is only in one direction. Spin can only be ↑ or ↓.

The calculations above for the y-direction spin vectors are shown explicitly below.

$$(0.707 \quad -.707i)\cdot\begin{pmatrix}.707\\.707i\end{pmatrix} = 1 \qquad (0.707 \quad .707i)\cdot\begin{pmatrix}.707\\-.707i\end{pmatrix} = 1 \qquad (0.707 \quad -.707i)\cdot\begin{pmatrix}.707\\-.707i\end{pmatrix} = 0$$

It is easy to show that **x- and z-spin states are not orthogonal** to one another. Any two different spin directions are not orthogonal. $\langle S_{xu}|S_{zu}\rangle = 0.707$, for example. **This is a 45° angle.**

$$\left(\overline{S_{xu}}\right)^T \cdot S_{zu} = 0.707 \quad \left(\overline{S_{xu}}\right)^T \cdot S_{zd} = 0.707 \quad \left(\overline{S_{xd}}\right)^T \cdot S_{zu} = 0.707 \quad \left(\overline{S_{xd}}\right)^T \cdot S_{zd} = -0.707$$

This of course means that, for example, $|S_{xu}\rangle$ and $|S_{xd}\rangle$ can be written as linear superpositions of $|S_{zu}\rangle$ and $|S_{zd}\rangle$, and $|S_{zu}\rangle$ and $|S_{zd}\rangle$ can be written as linear superpositions of $|S_{xu}\rangle$ and $|S_{xd}\rangle$.

$$S_{xu} = \begin{pmatrix} 0.707 \\ 0.707 \end{pmatrix} \quad \frac{1}{\sqrt{2}} \cdot S_{zu} + \frac{1}{\sqrt{2}} \cdot S_{zd} = \begin{pmatrix} 0.707 \\ 0.707 \end{pmatrix} \quad S_{xd} = \begin{pmatrix} 0.707 \\ -0.707 \end{pmatrix} \quad \frac{1}{\sqrt{2}} \cdot S_{zu} - \frac{1}{\sqrt{2}} \cdot S_{zd} = \begin{pmatrix} 0.707 \\ -0.707 \end{pmatrix}$$

$$S_{zu} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \frac{1}{\sqrt{2}} \cdot S_{xu} + \frac{1}{\sqrt{2}} \cdot S_{xd} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad S_{zd} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad \frac{1}{\sqrt{2}} \cdot S_{xu} - \frac{1}{\sqrt{2}} \cdot S_{xd} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

The concept of the linear superposition is central in quantum theory and has no classical analog. For example, if by measurement an electron is found to have spin-up in the z-direction, this means that the electron does not have a definite spin in either the x- or the y-direction because $|S_{zu}\rangle$ is a linear superposition of the x- and y-direction spin states.

$$S_{zu} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \frac{1}{\sqrt{2}} \cdot S_{xu} + \frac{1}{\sqrt{2}} \cdot S_{xd} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \frac{1}{\sqrt{2}} \cdot S_{yu} + \frac{1}{\sqrt{2}} \cdot S_{yd} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

In spite of its appearance, **a linear superposition is not a mixture**. In other words $|S_{zu}\rangle$ is not 50% $|S_{xu}\rangle$ and 50% $|S_{xd}\rangle$, or 50% $|S_{yu}\rangle$ and 50% $|S_{yd}\rangle$.

Another central dogma of quantum theory is that the wavefunction or state vector contains all the physical information available for the system. Quantum mechanics therefore consists, in large part, of extracting physical information from the wavefunction or state vector. Quantum mechanics consists of a small set of rules for carrying this procedure out mathematically.

For every observable of the system there is an operator. Since electrons can spin in the x-, y-, or z-directions, there are spin operators in those directions, or for that matter in any other arbitrary direction you might think of. In quantum mechanics **states are vectors and operators are matrices.** The spin operators in units of $h/4\pi$ are shown below. Note that squaring these operators gives the identity operator.

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

$$S_x^{\,2} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad S_y^{\,2} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad S_z^{\,2} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

For example, the square of the total spin operator in units of $h/4\pi$ is

$$S_{xyz} := S_x^{\,2} + S_y^{\,2} + S_z^{\,2} \qquad S_{xyz} = \begin{pmatrix} 3 & 0 \\ 0 & 3 \end{pmatrix}$$

A measurement operator extracts information about the system by operating on the wavefunction or state vector. One possible outcome is that the operation returns the state vector multiplied by a numerical constant. For example,

$$S_x \cdot S_{xu} = \begin{pmatrix} 0.707 \\ 0.707 \end{pmatrix} \qquad S_x \cdot S_{xd} = \begin{pmatrix} -0.707 \\ 0.707 \end{pmatrix} \qquad S_y \cdot S_{yu} = \begin{pmatrix} 0.707 \\ 0.707i \end{pmatrix} \qquad S_y \cdot S_{yd} = \begin{pmatrix} -0.707 \\ 0.707i \end{pmatrix}$$

$$S_z \cdot S_{zu} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad S_z \cdot S_{zd} = \begin{pmatrix} 0 \\ -1 \end{pmatrix} \qquad \text{or, for example:} \qquad \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \cdot \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ -1 \end{pmatrix}$$

In Dirac notation we would summarize these calculations as follows: $\mathbf{S_x}|S_{xu}\rangle = +1|S_{xu}\rangle$, $\mathbf{S_x}|S_{xd}\rangle = -1|S_{xd}\rangle$, $\mathbf{S_y}|S_{yu}\rangle = +1|S_{yu}\rangle$, $\mathbf{S_y}|S_{yd}\rangle = -1|S_{yd}\rangle$, $\mathbf{S_z}|S_{zu}\rangle = +1|S_{zu}\rangle$, $\mathbf{S_z}|S_{zd}\rangle = -1|S_{zd}\rangle$. In each of these cases, the state vector is an eigenfunction of the measurement operator with eigenvalue of either +1 or -1 (in units of $h/4\pi$). We say, for example, that $|S_{xu}\rangle$ is an eigenfunction of $\mathbf{S_x}$ with eigenvalue +1. The electron has a well-defined value for spin in the x-direction (spin-up) and subsequent measurements of the x-direction spin will yield the value of +1 as long as no intervening measurements in another spin direction are made.

The other possible outcome of the measurement operation is that it yields another state vector.

$$S_x \cdot S_{yu} = \begin{pmatrix} 0.707i \\ 0.707 \end{pmatrix} \qquad S_x \cdot S_{yd} = \begin{pmatrix} -0.707i \\ 0.707 \end{pmatrix} \qquad S_x \cdot S_{zu} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \qquad S_x \cdot S_{zd} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$S_y \cdot S_{xu} = \begin{pmatrix} -0.707i \\ 0.707i \end{pmatrix} \qquad S_y \cdot S_{xd} = \begin{pmatrix} 0.707i \\ 0.707i \end{pmatrix} \qquad S_y \cdot S_{zu} = \begin{pmatrix} 0 \\ i \end{pmatrix} \qquad S_y \cdot S_{zd} = \begin{pmatrix} -i \\ 0 \end{pmatrix}$$

$$S_z \cdot S_{xu} = \begin{pmatrix} 0.707 \\ -0.707 \end{pmatrix} \qquad S_z \cdot S_{xd} = \begin{pmatrix} 0.707 \\ 0.707 \end{pmatrix} \qquad S_z \cdot S_{yu} = \begin{pmatrix} 0.707 \\ -0.707i \end{pmatrix} \qquad S_z \cdot S_{yd} = \begin{pmatrix} 0.707 \\ 0.707i \end{pmatrix}$$

In Dirac notation these operations appear as: $\mathbf{S_x}|S_{yu}\rangle = i|S_{yd}\rangle$, $\mathbf{S_x}|S_{yd}\rangle = -i|S_{yu}\rangle$, $\mathbf{S_x}|S_{zu}\rangle = |S_{zd}\rangle$, $\mathbf{S_x}|S_{zd}\rangle = |S_{zu}\rangle$, etc. In each case the resulting vector is different than the vector operated on. We say, for example, $|S_{yu}\rangle$ is not an eigenfunction of $\mathbf{S_x}$, and therefore an electron in this state does not have a definite value for spin in the x-direction. X-direction spin measurements on a system known to be in state $|S_{yu}\rangle$ will yield completely random results.

To put it another way, quantum mechanical principles state that a system can be in a well-defined state, $|S_{yu}\rangle$, and yet the outcome of all experiments are not uniquely determined. While a measurement of spin in the y-direction will yield a predictable result, +1, measurement of spin in the x- or z-direction is completely unpredictable and all we can calculate is the average value, or expectation value for a large number of measurements. This is completely different than classical physics where if you know the state of the system, you know the values of all physical observables.

As another example, consider the ground state of the hydrogen atom for which the electron's wave function is $\Psi = \pi^{-1/2} \exp(-r)$. When the electron is in this state it has a precise energy, but not a well-defined position or momentum. This, of course, makes the concept of an electron trajectory impossible and it is, therefore, meaningless to think of the electron as moving in any traditional sense.

The quantum mechanical algorithm for calculating the expectation value is to execute the following matrix multiplication: <State Vector|**Operator**|State Vector>. This formalism is quite general and can be used whether the state vector is an eigenfunction of the operator or not. This is demonstrated below for the spin states that we have been studying.

$$\left(\overline{S_{xu}}\right)^T \cdot S_x \cdot S_{xu} = 1 \qquad \left(\overline{S_{xd}}\right)^T \cdot S_x \cdot S_{xd} = -1 \qquad \left(\overline{S_{zu}}\right)^T \cdot S_x \cdot S_{zu} = 0$$

$$\left(\overline{S_{zd}}\right)^T \cdot S_x \cdot S_{zd} = 0 \qquad \left(\overline{S_{yu}}\right)^T \cdot S_x \cdot S_{yu} = 0 \qquad \left(\overline{S_{yd}}\right)^T \cdot S_x \cdot S_{yd} = 0$$

$$\left(\overline{S_{xu}}\right)^T \cdot S_y \cdot S_{xu} = 0 \qquad \left(\overline{S_{xd}}\right)^T \cdot S_y \cdot S_{xd} = 0 \qquad \left(\overline{S_{zu}}\right)^T \cdot S_y \cdot S_{zu} = 0$$

$$\left(\overline{S_{zd}}\right)^T \cdot S_y \cdot S_{zd} = 0 \qquad \left(\overline{S_{yu}}\right)^T \cdot S_y \cdot S_{yu} = 1 \qquad \left(\overline{S_{yd}}\right)^T \cdot S_y \cdot S_{yd} = -1$$

$$\left(\overline{S_{xu}}\right)^T \cdot S_z \cdot S_{xu} = 0 \qquad \left(\overline{S_{xd}}\right)^T \cdot S_z \cdot S_{xd} = 0 \qquad \left(\overline{S_{zu}}\right)^T \cdot S_z \cdot S_{zu} = 1$$

$$\left(\overline{S_{zd}}\right)^T \cdot S_z \cdot S_{zd} = -1 \qquad \left(\overline{S_{yu}}\right)^T \cdot S_z \cdot S_{yu} = 0 \qquad \left(\overline{S_{yd}}\right)^T \cdot S_z \cdot S_{yd} = 0$$

Let's look at the first six entries because they are representative of the remaining results. If the electron is in the state $|S_{xu}\rangle$ measurement of $\mathbf{S_x}$ will always yield the value of +1 (in units of h/4π). If the electron is in the state $|S_{xd}\rangle$ measurement of Sx will always yield the value of -1 (in units of h/4π). If instead $\mathbf{S_y}$ or $\mathbf{S_z}$ are measured, the measurement results will be a statistically random collection of +1 and -1, and the average value will, of course, be zero. Only when the system is in an eigenstate of the measurement operator is the outcome of the experiment certain.

This brings us to the concept of probability and how it is calculated in quantum mechanics. The projection of one state on to another, $\langle S_{zu}|S_{xd}\rangle = .707$, is a **probability amplitude**. Its absolute square, $\langle S_{xd}|S_{zu}\rangle\langle S_{zu}|S_{xd}\rangle = |\langle S_{zu}|S_{xd}\rangle|^2 = 0.5$ (remember $\langle S_{xd}|S_{zu}\rangle = \langle S_{zu}|S_{xd}\rangle^*$), is the **probability** that an electron in state $|S_{xd}\rangle$ will be found by measurement in the state $|S_{zu}\rangle$. Representative calculations are shown below.

$$\left[\left|\left(\overline{S_{zu}}\right)^T \cdot S_{xu}\right|\right]^2 = 0.5 \qquad \left[\left|\left(\overline{S_{zd}}\right)^T \cdot S_{xu}\right|\right]^2 = 0.5 \qquad \left[\left|\left(\overline{S_{xu}}\right)^T \cdot S_{yu}\right|\right]^2 = 0.5 \qquad \left[\left|\left(\overline{S_{xu}}\right)^T \cdot S_{zd}\right|\right]^2 = 0.5$$

Let's review these concepts by taking a specific example. The electron is in the state $|S_{xu}\rangle$ and we wish to measure $\mathbf{S_z}$. According to quantum mechanical procedures the average value for a statistically meaningful number of measurements is zero - $\langle S_{xu}|\mathbf{S_z}|S_{xu}\rangle = 0$. The eigenstates (eigenfunctions) for $\mathbf{S_z}$ are $|S_{zu}\rangle$ and $|S_{zd}\rangle$ with eigenvalues +1 and -1, respectively. As the first two entries above show, the probability that an electron in state $|S_{xu}\rangle$ will be found in $|S_{zu}\rangle$ with eigenvalue +1 is 0.5, and the probability that it will be found in state $|S_{zd}\rangle$ with eigenvalue -1 is 0.5. Thus, the **average value** is **expected** to be zero, and the two ways of determining the average or expectation value of a measurement are consistent and equivalent.

There is yet another way to look at this issue. In quantum mechanics for most pairs of observables the order of measurement is important. Quantum mechanical operators don't generally commute. For example, as shown below, $\mathbf{S_xS_y}|S_{zu}\rangle$ does not equal $\mathbf{S_yS_x}|S_{zu}\rangle$. This means that if the electron is in the state $|S_{zu}\rangle$ the combined operators $\mathbf{S_xS_y}$ and $\mathbf{S_yS_x}$ yield different measurement results.

$$S_x \cdot S_y \cdot S_{zu} = \begin{pmatrix} i \\ 0 \end{pmatrix} \qquad S_y \cdot S_x \cdot S_{zu} = \begin{pmatrix} -i \\ 0 \end{pmatrix} \qquad \left(S_x \cdot S_y - S_y \cdot S_x\right) \cdot S_{zu} = \begin{pmatrix} 2i \\ 0 \end{pmatrix}$$

Operators that do not commute have incompatible eigenstates. If a state vector is an eigenstate of one of the operators, it is not an eigenstate of the other. The fact that **Sx** and **Sy** do not commute means that an electron cannot simultaneously have well-defined values for S_x and S_y. It is not surprising that there is a deep connection between these properties of operators and the Uncertainty Principle. The commutators for the spin operators are shown below.

$$S_x \cdot S_y - S_y \cdot S_x = \begin{pmatrix} 2i & 0 \\ 0 & -2i \end{pmatrix} \qquad 2 \cdot i \cdot S_z = \begin{pmatrix} 2i & 0 \\ 0 & -2i \end{pmatrix} \qquad S_z \cdot S_x - S_x \cdot S_z = \begin{pmatrix} 0 & 2 \\ -2 & 0 \end{pmatrix}$$

$$S_y \cdot S_z - S_z \cdot S_y = \begin{pmatrix} 0 & 2i \\ 2i & 0 \end{pmatrix} \qquad 2 \cdot i \cdot S_x = \begin{pmatrix} 0 & 2i \\ 2i & 0 \end{pmatrix} \qquad 2 \cdot i \cdot S_y = \begin{pmatrix} 0 & 2 \\ -2 & 0 \end{pmatrix}$$

The Uncertainty Principle can also be illustrated by calculating ΔSx and ΔSy for an electron known to be in the Szu state. Since we are working in units of h/4π, the uncertainty relation is: $\Delta S_x \cdot \Delta S_y \geq 1.$

$$\sqrt{S_{zu}{}^T \cdot S_x \cdot S_x \cdot S_{zu} - \left(S_{zu}{}^T \cdot S_x \cdot S_{zu}\right)^2} \cdot \sqrt{S_{zu}{}^T \cdot S_y \cdot S_y \cdot S_{zu} - \left(S_{zu}{}^T \cdot S_y \cdot S_{zu}\right)^2} = 1$$

We have been dealing with matrix operators and their associated eigenvectors and eigenvalues. The eigenvectors and eigenvalues can be obtained from the matrix operators with Mathcad's **eigenvecs** and **eigenvals** commands as is shown below.

$$eigenvals(S_x) = \begin{pmatrix} 1 \\ -1 \end{pmatrix} \qquad eigenvec(S_x, 1) = \begin{pmatrix} 0.707 \\ 0.707 \end{pmatrix} \qquad eigenvec(S_x, -1) = \begin{pmatrix} -0.707 \\ 0.707 \end{pmatrix}$$

$$eigenvals(S_y) = \begin{pmatrix} 1 \\ -1 \end{pmatrix} \qquad eigenvecs(S_y) = \begin{pmatrix} -0.707i & 0.707 \\ 0.707 & -0.707i \end{pmatrix}$$

$$eigenvals(S_z) = \begin{pmatrix} 1 \\ -1 \end{pmatrix} \qquad eigenvecs(S_z) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

XIII. Visualizing the Difference Between a Superposition and Mixture

Tutorial: *LibreTexts Quantum Tutorials*

The superposition principle, as Feynman said, is at the heart of quantum mechanics. While its mathematical expression is simple, its true meaning is difficult to grasp. For example,

given a linear superposition (not normalized) of two states,

$$|\Psi\rangle = |\phi_1\rangle + |\phi_2\rangle$$

one might assume that it represents a mixture of ϕ_1 and ϕ_2. In other words, half of the quons are in state ϕ_1 and half in ϕ_2. However, the correct quantum mechanical interpretation of this equation is that the system represented by Ψ is **simultaneously in the states ϕ_1 and ϕ_2**, properly weighted.

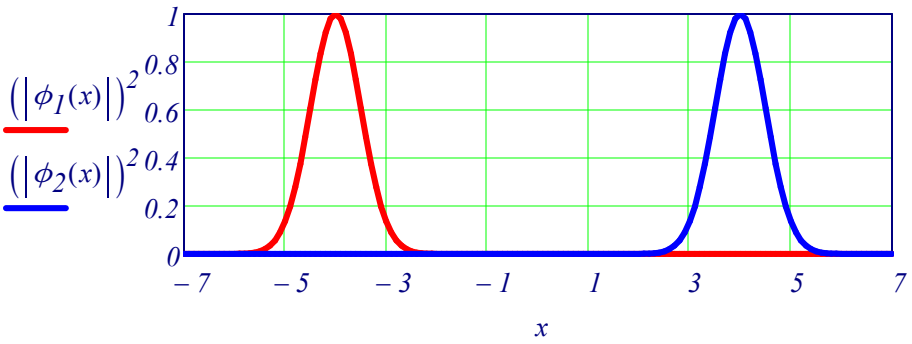
A mixture, half ϕ_1 and half ϕ_2, or any other ratio, **cannot be represented by a wavefunction**. It requires a **density operator**, which is a more general quantum mechanical construct that can be used to represent both pure states (superpositions) and mixtures, as shown below.

$$\hat{\rho}_{\max} = |\Psi\rangle\langle\Psi| \qquad \hat{\rho}_{\min d} = \sum p_i |\Psi_i\rangle\langle\Psi_i|$$

In the equation on the right, p_i is the fraction of the mixture in the state Ψ_i.

To illustrate how these equations distinguish between a mixture and a superposition, we will consider a superposition and a mixture of equally weighted gaussian functions representing one-dimensional wave packets. The normalization constants are omitted in the interest of mathematical clarity. The gaussians are centered at x = ± 4.

$$\phi_1(x) := \exp\left[-(x+4)^2\right] \qquad \phi_2(x) := \exp\left[-(x-4)^2\right] \qquad x := -7, -6.9 .. 7$$



To visualize how the density operator discriminates between a superposition and a mixture, we calculate its matrix elements in coordinate space for the **50-50 superposition** and **mixture of ϕ_1 and ϕ_2**.

The superposition is considered first.

$$\Psi(x) := \phi_1(x) + \phi_2(x)$$

The matrix elements of this pure state are calculated as follows.

$$\rho_{\text{pure}} = \langle x|\hat{\rho}_{\text{pure}}|x'\rangle = \langle x|\Psi\rangle\,\langle\Psi|x'\rangle$$

Looking at the right side we see that the matrix elements are the **product of the probability amplitudes** of a quon in state being at x and x′. Next we display the density matrix graphically.

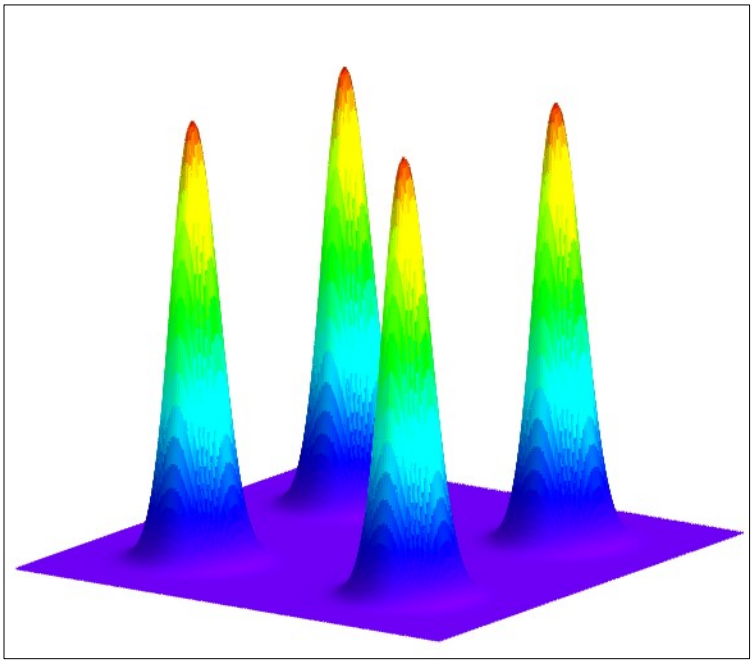
Density Matrix Pure Superposition State

$$DensityMatrixPure(x_1, x_2) := \Psi(x_1) \cdot \Psi(x_2)$$

$$x_0 := 8 \qquad N := 160 \qquad i := 0..N \qquad j := 0..N$$

$$x1_i := -x_0 + \frac{2 \cdot x_0 \cdot i}{N} \qquad x2_j := -x_0 + \frac{2 \cdot x_0 \cdot j}{N}$$

$$DensityMatrixPure_{i,j} := DensityMatrixPure(x1_i, x2_j)$$



DensityMatrixPure

The presence of off-diagonal elements in this density matrix is the signature of a quantum mechanical superposition. For example,from the quantum mechanical perspective bi-location is possible.

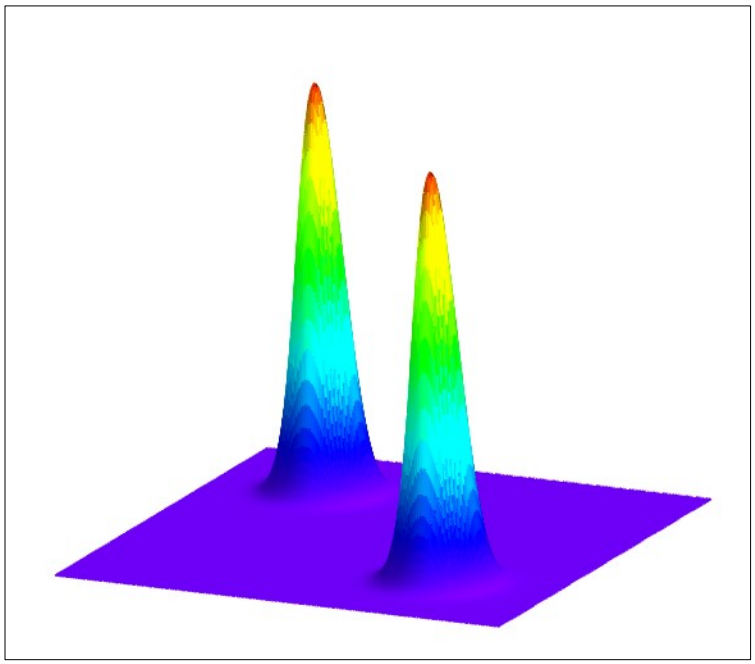
Now we turn our attention to the density matrix of a mixture of gaussian states.

Density Matrix of Mixture State

$$\rho_{\text{mix}} = \langle x | \hat{\rho}_{\text{mix}} | x' \rangle = \sum_i p_i \langle x|\phi_i\rangle \langle \phi_i|x'\rangle = \frac{1}{2}\langle x|\phi_1\rangle \langle \phi_1|x'\rangle + \frac{1}{2}\langle x|\phi_2\rangle \langle \phi_2|x'\rangle$$

$$DensityMatrixMix(x_1, x_2) := \frac{\phi_1(x_1)\cdot\phi_1(x_2) + \phi_2(x_1)\cdot\phi_2(x_2)}{2}$$

$$DensityMatrixMix_{i,j} := DensityMatrixMix(x1_i, x2_j)$$



DensityMatrixMix

The obvious difference between a superposition and a mixture is the
absence of off-diagonal elements,

$\phi_1(x_1)\cdot\phi_1(x_2) + \phi_2(x_1)\cdot\phi_2(x_2)$ in the mixed state.

This indicates the mixture is in a definite but unknown state; it is an example of classical ignorance.

An equivalent way to describe the difference between a superposition and a mixture, is to say that to calculate the probability of measurement outcomes
for a **superposition** you **add the probability amplitudes and square the sum**.
For a **mixture** you **square the individual probability amplitudes** and **sum the squares.**

Nick Herbert (Quantum Reality, page 64) suggested "quon" be used to stand for a generic quantum object. "A quon is any entity, no matter how immense, that exhibits both wave and particle aspects in the peculiar quantum manner.

Visualizing the Difference Between a Superposition and a Mixture - Continued

The Wigner function (**See Section XXIV**) can be used to illustrate the difference between a superposition and a mixture. First consider the following **linear superposition** of Gaussian functions.

$$\Psi(x) := \exp\left[-(x-5)^2\right] + \exp\left[-(x+5)^2\right]$$

The Wigner distribution (See Section XXIV) for this function is calculated and plotted below.

$$W(x,p) := \int_{-\infty}^{\infty} \left[\exp\left[-\left(x+\frac{s}{2}-5\right)^2\right] + \exp\left[-\left(x+\frac{s}{2}+5\right)^2\right]\right] \cdot \exp(i\cdot p\cdot s) \cdot \left[\exp\left[-\left(x-\frac{s}{2}-5\right)^2\right] + \exp\left[-\left(x-\frac{s}{2}+5\right)^2\right]\right] ds$$

Integration yields:

$$W(x,p) := \sqrt{2}\cdot\sqrt{\pi}\cdot\left(\begin{array}{l} 2\cdot\exp\left(-2\cdot x^2 - \frac{1}{2}\cdot p^2\right)\cdot\cos(10\cdot p) + \exp\left(-2\cdot x^2 + 20\cdot x - 50 - \frac{1}{2}\cdot p^2\right) \ldots \\ + \exp\left(-2\cdot x^2 - 20\cdot x - 50 - \frac{1}{2}\cdot p^2\right) \end{array}\right)$$

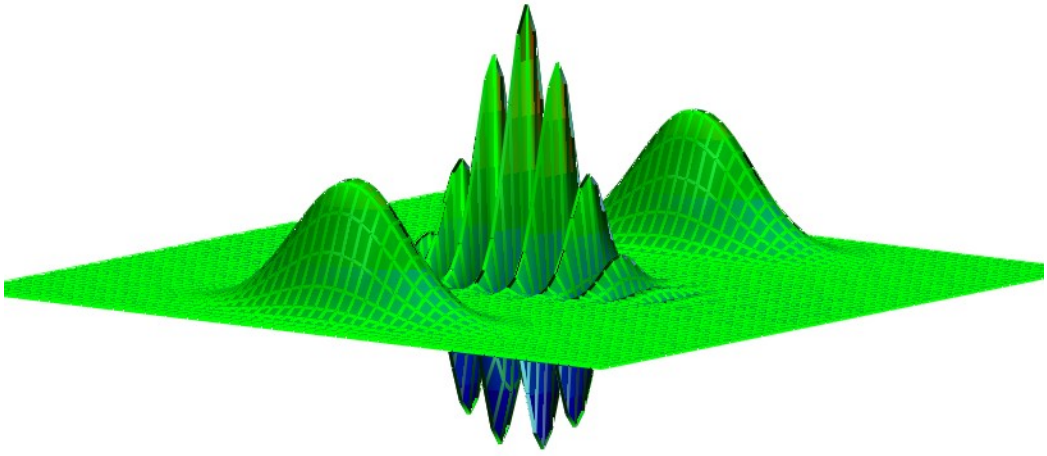
$$N := 60 \quad i := 0..N \quad x_i := -7 + \frac{14\cdot i}{N}$$

$$j := 0..N \quad p_j := -6 + \frac{12\cdot j}{N}$$

$$Wigner_{i,j} := W\left(x_i, p_j\right)$$

The signature of a superposition

the occurrence of interference fringes as seen in the center of the figure below.



Wigner

XIV. Two-Photon Interference

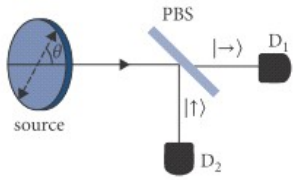
Polarization Beam Splitter and Pockel Cell

Tutorial: *Quantum Mechanics for Beginners,* M. Suhail Zubairy, Chapter 9.5

In this section, we discuss how we can measure the polarization state. A polarizer is an inconvenient device as the photon is either transmitted or it is absorbed. What is more desirable is a device that is able to send one polarization state (say $|\rightarrow\rangle$) along one way and the other $|\uparrow\rangle$ along a different path. This is done in a polarization beam splitter.

Let us consider a photon that is prepared in the polarization state

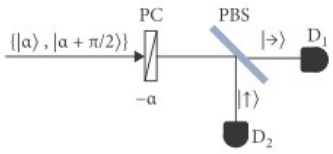
$$|\theta\rangle = \cos\theta\,|\rightarrow\rangle + \sin\theta\,|\uparrow\rangle.$$



If a photon polarized in a direction making an angle θ with the polarization axis is incident on a polarization beam splitter (PBS), it can pass through as a photon in state $|\rightarrow\rangle$ in the forward direction or get reflected in state $|\uparrow\rangle$ in the downward direction.

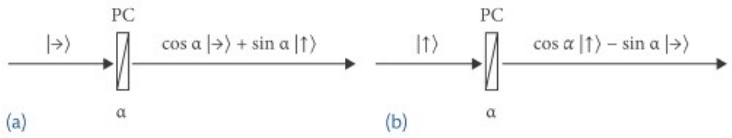
When such a photon is incident on a polarization beam splitter, as shown in the above figure, it can either go in the forward direction in the horizontally polarized state $|\rightarrow\rangle$ or in the downward direction in the vertically polarized state $|\uparrow\rangle$. We can then find the state of the photon depending on whether we get a click at the detector D1 or at the detector D2 . A click at D1 means that the photon is in the state $|\rightarrow\rangle$ and a click at D2 means that the photon is in the state $|\uparrow\rangle$. The probability of the click at D1 is $|\langle\rightarrow|\theta\rangle|^2 = \cos^2\theta$ and the probability of click at D2 is $|\langle\uparrow|\theta\rangle|^2 = \sin^2\theta$.

Unlike a polarizer, the polarizing beam splitter cannot be easily rotated to measure the polarization state along some other axis, say along an axis rotated by an angle α with the horizontal. For that, we need to insert a polarization rotator before the polarizing beam splitter. This device should be able to rotate the state of the polarization of an incoming photon by an angle α before passing it through the polarization beam splitter.



If a photon polarized in a direction making an angle θ with the polarization axis is incident on a polarization beam splitter (PBS), it can pass through as a photon in state $|\rightarrow\rangle$ in the forward direction or get reflected in state $|\uparrow\rangle$ in the downward direction.

One such device is the Pockel cell. It is an electro-optic device which rotates the polarization of the incident light passing



A Pockel cell that rotates the polarization by angle $-\alpha$ followed by a beam splitter can determine the polarization of the incoming photon. A click at D1 implies that the polarization of the incoming photon is along an angle α with the horizontal and a click at D2 means that the state of the incoming photon is along an angle $\alpha + \pi/2$ with the horizontal.

through it in proportion to the applied voltage. As an example, by applying an appropriate voltage, the Pockel cell can rotate the polarization of a photon by an angle α with the horizontal as shown in . As a result the horizontally and vertically polarized photons in states $|\rightarrow\rangle$ and $|\uparrow\rangle$, respectively, undergo the following transformations:

$$|\rightarrow\rangle \rightarrow |+\alpha\rangle \equiv |\,\alpha\,\rangle = \cos\alpha\,|\rightarrow\rangle + \sin\alpha\,|\uparrow\rangle$$
$$|\uparrow\rangle \rightarrow |-\alpha\rangle \equiv |\,\alpha + \pi/2\,\rangle = \cos\alpha\,|\uparrow\rangle - \sin\alpha\,|\rightarrow\rangle.$$

We note that, just like the pair of states $\{|\rightarrow\rangle, |\uparrow\rangle\}$, the states $\{|+\alpha\,\rangle, |-\alpha\rangle\}$ are normalized and are mutually orthogonal, i.e.,

$$\langle+\alpha\,|\,+\alpha\,\rangle = \langle-\alpha\,|\,-\alpha\,\rangle = 1,$$
$$\langle+\alpha\,|\,-\alpha\,\rangle = \langle-\alpha\,|\,+\alpha\,\rangle = 0.$$

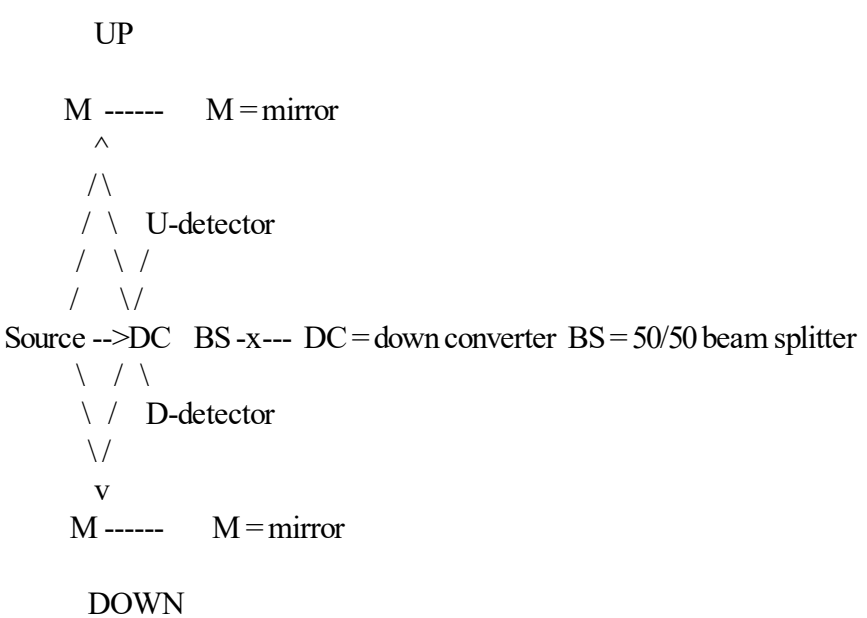
A polarization beam splitter can determine whether the polarization state of the incoming photon is $|\rightarrow\rangle$ or $|\uparrow\rangle$. A question of interest is: How can we determine whether the polarization of the incoming photon is along an angle α or along $\alpha + \pi/2$ with the horizontal? The corresponding states are $|+\alpha\,\rangle \equiv |\alpha\rangle$ and $|-\alpha\,\rangle \equiv |\,\alpha + \pi/2\rangle$. A way of doing this is to first rotate the polarization angle of the incoming photon by an angle $-\alpha$. This should transform the state $|\alpha\rangle$ to $|\rightarrow\rangle$ and the state $|\alpha + \pi/2\rangle$ to $|\uparrow\rangle$. This can be done by passing the photon through a Pockel cell that rotates the polarization by an angle $-\alpha$ with the horizontal. Next the photon passes through a polarization beam splitter as shown in the Figure below. If the detector D1 clicks, the polarization of the incoming photon is along an angle α with the horizontal (in state $|\alpha\rangle$) and a click at the detector D 2 means that the state of the incoming photon is along an angle $\alpha + \pi/2$ with the horizontal (in state $|\alpha + \pi/2\rangle$).

As an example, if we want to find whether the photon is in the state $|\,\theta = 45^\circ\,\rangle \equiv |\nearrow\rangle$ or $|\,\theta = 135^\circ\,\rangle \equiv |\nwarrow\rangle$, we consider the set-up in Fig. 9.14 with $\alpha = 45^\circ$. A rotation of the polarization by an angle -45° transforms the state $|\theta = 45^\circ\,\rangle \equiv |\nearrow\rangle$ to the horizontally polarized state $|\rightarrow\rangle$ and the state $|\theta = 135^\circ\,\rangle \equiv |\nwarrow\rangle$ to the vertically polarized state $|\uparrow\rangle$. Therefore a click at D1 implies that the incoming photon is in the state $|\nearrow\rangle$ and a click at D2 implies that the incoming photon is in the state $|\nwarrow\rangle$.

Two-Photon Interference

Math: *Physical_and_Theoretical_Chemistry,* Dr. Frank Rioux
Reference: Greenberger, D.M.; Horne, M.A.; Zeilinger, A. *Physics Today*, **1993**, *44(8)*, 22.

In this experiment a down converter, DC, transforms an incident photon into two lower energy photons. One photon takes the upper path and the other the lower path or vice versa. The results of this experiment are that both photons are detected at either U or D. One photon is never detected at U while the other is detected at D. A quantum mechanical analysis of this phenomena is provided below.



Orthonormal basis states:

Photon moving in up-direction: $u := \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ $(u)^T \cdot u = 1$

Photon moving in down-direction: $d := \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ $(d)^T \cdot d = 1$ $(u)^T \cdot d = 0$

Operators:

Operator for interaction with the mirror: $M := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

Operator for interaction with a 50/50 beam splitter: $BS := \frac{1}{\sqrt{2}} \cdot \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}$

A 90^o phase shift between transmission and reflection at the beam splitter is required to satisfy energy conservation. By convention the phase shift is assigned to reflection.

The down-converter creates the following entangled state:

$$|\Psi_b\rangle = [|u\rangle_1|d\rangle_2 + |d\rangle_1|u\rangle_2]/2^{1/2}$$

This is a symmetric state because photons are bosons.

After creation in the down-converter, both photons interact with a mirror and a beam splitter before reaching a detector, either U or D. To be detected at the U-detector the photon must be moving in the up-direction (photon state = |u>). To be detected at the D-detector the photon must be moving in the down-direction (photon state = |d>). The probabilities for the four possible experimental outcomes are calculated below.

Both photons arrive at the U-detector: $|_1\langle u|_2\langle u|\mathbf{BS}\,\mathbf{M}|\Psi_b\rangle|^2$

$$\left[\left|\frac{\left[(u)^T\cdot BS\cdot M\cdot u\right]\cdot\left[(u)^T\cdot BS\cdot M\cdot d\right]+\left[(u)^T\cdot BS\cdot M\cdot d\right]\cdot\left[(u)^T\cdot BS\cdot M\cdot u\right]}{\sqrt{2}}\right|\right]^2 = 0.5$$

Both photons arrive at the D-detector: $|_1\langle d|_2\langle d|\mathbf{BS}\,\mathbf{M}|\Psi_b\rangle|^2$

$$\left[\left|\frac{\left[(d)^T\cdot BS\cdot M\cdot u\right]\cdot\left[(d)^T\cdot BS\cdot M\cdot d\right]+\left[(d)^T\cdot BS\cdot M\cdot d\right]\cdot\left[(d)^T\cdot BS\cdot M\cdot u\right]}{\sqrt{2}}\right|\right]^2 = 0.5$$

Photon 1 arrives at the U-detector and photon 2 arrives at the D-detector: $|_1\langle u|_2\langle d|\mathbf{BS}\,\mathbf{M}|\Psi_b\rangle|^2$

$$\left[\left|\frac{\left[(u)^T\cdot BS\cdot M\cdot u\right]\cdot\left[(d)^T\cdot BS\cdot M\cdot d\right]+\left[(u)^T\cdot BS\cdot M\cdot d\right]\cdot\left[(d)^T\cdot BS\cdot M\cdot u\right]}{\sqrt{2}}\right|\right]^2 = 0$$

Photon 1 arrives at the D-detector and photon 2 arrives at the U-detector: $|_1\langle d|_2\langle u|\mathbf{BS}\,\mathbf{M}|\Psi_b\rangle|^2$

$$\left[\left|\frac{\left[(d)^T\cdot BS\cdot M\cdot u\right]\cdot\left[(u)^T\cdot BS\cdot M\cdot d\right]+\left[(d)^T\cdot BS\cdot M\cdot d\right]\cdot\left[(u)^T\cdot BS\cdot M\cdot u\right]}{\sqrt{2}}\right|\right]^2 = 0$$

If the experiment could be performed with fermions, they would be created in the following anti-symmetric entangled state:

$$|\Psi_f\rangle = [|u\rangle_1|d\rangle_2 - |d\rangle_1|u\rangle_2]/2^{1/2}$$

As the analysis below shows, the results for fermions would be exactly opposite to those for bosons. Two fermions would never arrive at the same detector.

Both fermions arrive at the U-detector: $|_1\langle u|_2\langle u|\mathbf{BS\,M}|\Psi_f\rangle|^2$

$$\left[\left|\frac{\left[(u)^T\cdot BS\cdot M\cdot u\right]\cdot\left[(u)^T\cdot BS\cdot M\cdot d\right]-\left[(u)^T\cdot BS\cdot M\cdot d\right]\cdot\left[(u)^T\cdot BS\cdot M\cdot u\right]}{\sqrt{2}}\right|\right]^2 = 0 \quad \text{<==Interference}$$

Both fermions arrive at the D-detector: $|_1\langle d|_2\langle d|\mathbf{BS\,M}|\Psi_f\rangle|^2$

$$\left[\left|\frac{\left[(d)^T\cdot BS\cdot M\cdot u\right]\cdot\left[(d)^T\cdot BS\cdot M\cdot d\right]-\left[(d)^T\cdot BS\cdot M\cdot d\right]\cdot\left[(d)^T\cdot BS\cdot M\cdot u\right]}{\sqrt{2}}\right|\right]^2 = 0 \quad \text{<==Interference}$$

Fermion 1 arrives at the U-detector and fermion 2 arrives at the D-detector: $|_1\langle u|_2\langle d|\mathbf{BS\,M}|\Psi_f\rangle|^2$

$$\left[\left|\frac{\left[(u)^T\cdot BS\cdot M\cdot u\right]\cdot\left[(d)^T\cdot BS\cdot M\cdot d\right]-\left[(u)^T\cdot BS\cdot M\cdot d\right]\cdot\left[(d)^T\cdot BS\cdot M\cdot u\right]}{\sqrt{2}}\right|\right]^2 = 0.5$$

Fermion 1 arrives at the D-detector and fermion 2 arrives at the U-detector: $|_1\langle d|_2\langle u|\mathbf{BS\,M}|\Psi_f\rangle|^2$

$$\left[\left|\frac{\left[(d)^T\cdot BS\cdot M\cdot u\right]\cdot\left[(u)^T\cdot BS\cdot M\cdot d\right]-\left[(d)^T\cdot BS\cdot M\cdot d\right]\cdot\left[(u)^T\cdot BS\cdot M\cdot u\right]}{\sqrt{2}}\right|\right]^2 = 0.5$$

The results of this tutorial enable us to formulate a sociology for bosons and fermions: bosons are gregarious and enjoy companionship; fermions are anti-social and prefer solitude.

But why do bosons always end up at the same detector and fermions (hypothetically) always end up at different detectors? Why in both cases do half of the possible outcomes not occur? Are the bosons and fermions interfering with each other directly? Is there a subtle attractive interaction between bosons and an equally subtle, non-electrostatic, repulsive interaction between fermions?

Not according to Roy Glauber who said,
"**The things that interfere in quantum mechanics are not particles**.
They are probability amplitudes for certain events.
It is the fact that **probability amplitudes add up like complex numbers that accounts for all quantum mechanical interferences**."
[American Journal of Physics **63**, 12 (1995)]

The analysis used in this tutorial clearly illustrates Glauber's assertion.

Reference: Greenberger, D.M.; Horne, M.A.; Zeilinger, A. *Physics Today*, **1993**, *44(8)*, 22.

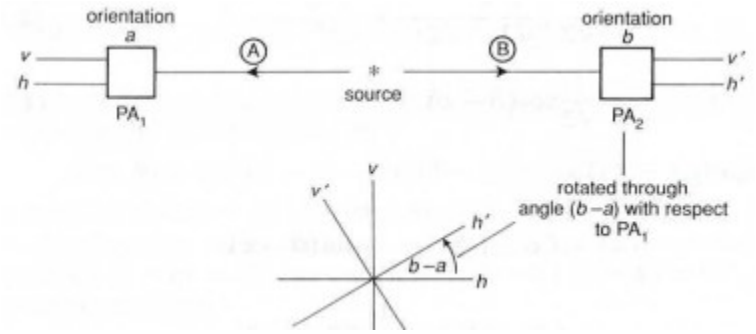
XV. A Proof of Bell's Theorem

This Analysis is Based Jim Baggott's analysis of Bell's theorem as presented in Chapter 4 of ***The Meaning of Quantum Theory*** & Dr. Frank Rioux's Methodology using matrix and tensor algebra.

A two-stage atomic cascade emits entangled photons (A and B) in opposite directions with the same circular polarization according to observers in their path.

$$|\Psi\rangle = \frac{1}{\sqrt{2}}\left[|L\rangle_A|L\rangle_B + |R\rangle_A|R\rangle_B\right]$$

The experiment involves the measurement of photon polarization states in the vertical/horizontal measurement basis, and allows for the rotation of the right-hand detector through an angle of θ, in order to explore the consequences of quantum mechanical entanglement. PA stands for polarization analyzer and could simply be a calcite crystal.



In vector notation the left- and right-circular polarization states are expressed as follows:

Left circular polarization: $L := \frac{1}{\sqrt{2}} \cdot \begin{pmatrix} 1 \\ i \end{pmatrix}$ Right circular polarization: $R := \frac{1}{\sqrt{2}} \cdot \begin{pmatrix} 1 \\ -i \end{pmatrix}$

Tensor Product of Column Vectors, In tensor notation the initial state is the following entangled superposition:

$$|\Psi\rangle = \frac{1}{\sqrt{2}}\left[|L\rangle_A|L\rangle_B + |R\rangle_A|R\rangle_B\right] = \frac{1}{2\sqrt{2}}\left[\begin{pmatrix}1\\i\end{pmatrix}_A \otimes \begin{pmatrix}1\\i\end{pmatrix}_B + \begin{pmatrix}1\\-i\end{pmatrix}_A \otimes \begin{pmatrix}1\\-i\end{pmatrix}_B\right] = \frac{1}{2\sqrt{2}}\left[\begin{pmatrix}1\\i\\i\\-1\end{pmatrix} + \begin{pmatrix}1\\-i\\-i\\-1\end{pmatrix}\right] = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\0\\-1\end{pmatrix}$$

However, as mentioned above, the photon polarization measurements will actually be made in the vertical/horizontal basis. These polarization measurement states for photons A and B in vector representation are given below. Θ is the angle through which the PA_2 has been rotated.

Vertical Polarization: $V_A := \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ $V_B := \begin{pmatrix} \cos(\theta) \\ -\sin(\theta) \end{pmatrix}$ Horizontal Polarization: $H_A := \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ $H_B := \begin{pmatrix} \sin(\theta) \\ \cos(\theta) \end{pmatrix}$

It is easy to show that |Ψ> in the vertical/horizontal basis is,

$$|\Psi\rangle = \frac{1}{\sqrt{2}}\left[|V\rangle_A|V\rangle_B - |H\rangle_A|H\rangle_B\right] = \frac{1}{2\sqrt{2}}\left[\begin{pmatrix}1\\0\end{pmatrix}_A \otimes \begin{pmatrix}1\\0\end{pmatrix}_B - \begin{pmatrix}0\\1\end{pmatrix}_A \otimes \begin{pmatrix}0\\1\end{pmatrix}_B\right] = \frac{1}{2\sqrt{2}}\left[\begin{pmatrix}1\\0\\0\\0\end{pmatrix} - \begin{pmatrix}0\\0\\0\\1\end{pmatrix}\right] = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\0\\-1\end{pmatrix}$$

There are four possible measurement outcomes: both photons are vertically polarized, both are horizontally polarized, one is vertical and the other horizontal, and vice versa. The vector representations of the measurement states are obtained by tensor multiplication of the individual photon states.

$$|V_A V_B\rangle = \begin{pmatrix}1\\0\end{pmatrix} \otimes \begin{pmatrix}\cos\theta\\-\sin\theta\end{pmatrix} = \begin{pmatrix}\cos\theta\\-\sin\theta\\0\\0\end{pmatrix} \qquad |V_A H_B\rangle = \begin{pmatrix}1\\0\end{pmatrix} \otimes \begin{pmatrix}\sin\theta\\\cos\theta\end{pmatrix} = \begin{pmatrix}\sin\theta\\\cos\theta\\0\\0\end{pmatrix}$$

$$|H_A V_B\rangle = \begin{pmatrix}0\\1\end{pmatrix} \otimes \begin{pmatrix}\cos\theta\\-\sin\theta\end{pmatrix} = \begin{pmatrix}0\\0\\\cos\theta\\-\sin\theta\end{pmatrix} \qquad |H_A H_B\rangle = \begin{pmatrix}0\\1\end{pmatrix} \otimes \begin{pmatrix}\sin\theta\\\cos\theta\end{pmatrix} = \begin{pmatrix}0\\0\\\sin\theta\\\cos\theta\end{pmatrix}$$

The initial state and the measurement eigenstates are written in Mathcad syntax.

$$\Psi := \frac{1}{\sqrt{2}} \cdot \begin{pmatrix}1\\0\\0\\-1\end{pmatrix}$$

$$VaVb(\theta) := \begin{pmatrix}cos(\theta)\\-sin(\theta)\\0\\0\end{pmatrix} \qquad VaHb(\theta) := \begin{pmatrix}sin(\theta)\\cos(\theta)\\0\\0\end{pmatrix}$$

$$HaVb(\theta) := \begin{pmatrix}0\\0\\cos(\theta)\\-sin(\theta)\end{pmatrix} \qquad HaHb(\theta) := \begin{pmatrix}0\\0\\sin(\theta)\\cos(\theta)\end{pmatrix}$$

The projections of the initial state onto the four measurement states are,

Note: θ.dot --> $\theta := \pi$

Probability Amplitude:

$$\begin{pmatrix}VaVb(\theta)^T \cdot \Psi\\VaHb(\theta)^T \cdot \Psi\\HaVb(\theta)^T \cdot \Psi\\HaHb(\theta)^T \cdot \Psi\end{pmatrix} \rightarrow \begin{pmatrix}-\frac{\sqrt{2}}{2}\\0\\0\\\frac{\sqrt{2}}{2}\end{pmatrix}$$

Probability:

$$\begin{bmatrix}\left(VaVb(\theta)^T \cdot \Psi\right)^2\\\left(VaHb(\theta)^T \cdot \Psi\right)^2\\\left(HaVb(\theta)^T \cdot \Psi\right)^2\\\left(HaHb(\theta)^T \cdot \Psi\right)^2\end{bmatrix} \rightarrow \begin{pmatrix}\frac{1}{2}\\0\\0\\\frac{1}{2}\end{pmatrix}$$

Assigning an eigenvalue of +1 to a vertical polarization measurement and -1 to a horizontal polarization measurement allows the calculation of the expectation value for the joint polarization measurements, a function which quantifies the correlation between the joint measurements. The eigenvalues for the four joint measurement outcomes are: VaVb = 1; VaHb = -1; HaVb = -1; HaHb = 1. Weighting these by the probability of their occurrence gives the **Expectation Value, E(θ)** or **Correlation Function.**

$$E(\theta) := \left(VaVb(\theta)^T \cdot \Psi\right)^2 - \left(VaHb(\theta)^T \cdot \Psi\right)^2 - \left(HaVb(\theta)^T \cdot \Psi\right)^2 + \left(HaHb(\theta)^T \cdot \Psi\right)^2 \rightarrow \cos(\theta)^2 - \sin(\theta)^2 \rightarrow \cos(2\cdot\theta)$$

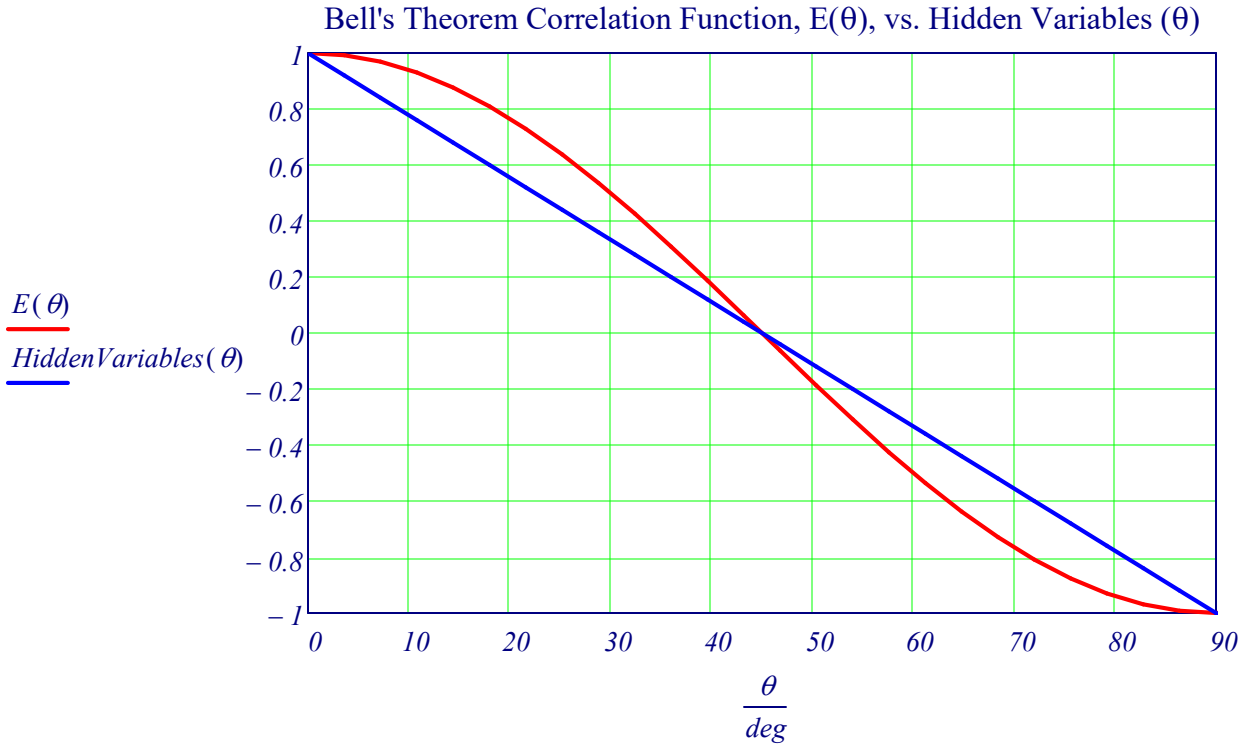
As shown above the evaluation of E(θ) yields cos(2θ). For $\theta = 0^0$ there is perfect correlation; for $\theta = 90^0$ perfect anti-correlation; for $\theta = 45^0$ no correlation.

$$E(0\cdot deg) = 1 \qquad E(90\cdot deg) = -1 \qquad E(45\cdot deg) = 0$$

Baggott presented a correlation function for this experiment based on a local hidden variable model of reality (pp. 110-113, 127-131). It (linear blue line) and the quantum mechanical correlation function, E(θ), are compared on the graph below. Quantum theory and local realism disagree at all angles except 0, 45, and 90 degrees.

$$HiddenVariables(\theta) := 1 - \frac{\theta}{45deg}$$

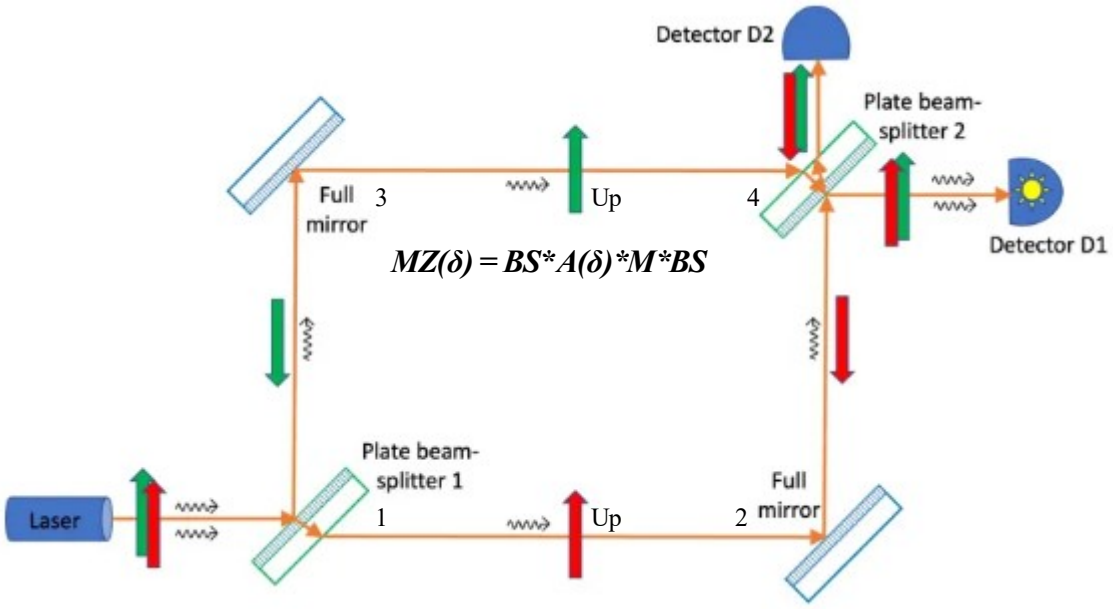
Comparison of Quantum Theory Expectation vs. Local Hidden Variables



XIV. Quantitative Analysis of Phase Splitting on Mach-Zehnder Inferometer

Graphics: https://quantumphysics-consciousness.eu/index.php/en/the-mach-zehnder-interferometer-explained/

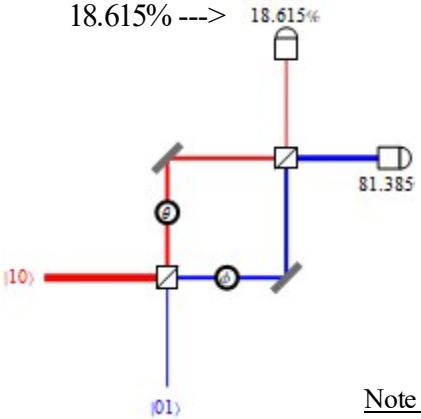
A wave can experience a phase shift (δ) upon full or partial reflection. This is a feature that is applied in the Mach-Zehnder interferometer, MZ, to induce phase differences in split light waves en thus invoke interference effects when they are combined again. Mach-Zehnder interferometer beam splitters (BS) are used to achieve several things:
*split a light beam in two equal and synchronous beams, a reflected beam and a strait-through passing beam,
*induce a phase (δ) shift in the reflected beam. NB: The strait-through passing beam does not experience phase shift.
*recombine the two light beams in order to let them interfere.

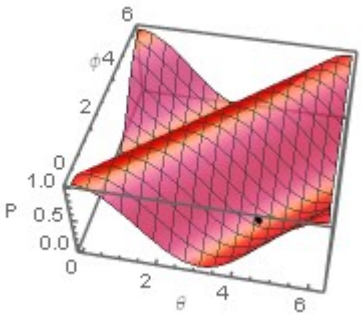


Now we follow the waves that should reach detector D2. The Up wave traveling along 1-2-4 receives a 180° phase shift at beam splitter (BS) 1. Another 180° phase shift (δ) at full mirror 2. Then finally zero phase shift by the reflection from glass by Mirror (M) to air at beam splitter 4 in the direction of D2. Total is thus 360°. The wave D traveling along 1-3-4 receives only one phase shift at mirror 3 of 180°. So the recombined two waves going from beam splitter 4 to detector D2 will interfere with phase difference 180°, which means fully opposite phases. Which means destructive interference. D2 receives no light.

Mathematica: 3D Solution of Beam Probability with Relative Phase Shifts θ and ϕ.

18.615% ---> 18.615%





Note P, θ, ϕ Location of above black dot.

Probability of going into top detector: P_{top}

$$P_{top}(\theta,\phi) := \cos\left(\frac{\theta-\phi}{2}\right)^2$$

$$P_{top}(2.24938,0) = 18.615\cdot\%$$

beam splitter		$\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}$
mirror		$\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$
phase shifter		$\begin{pmatrix}e^{i\theta} & 0\\ 0 & e^{i\phi}\end{pmatrix}$

XVII. Simulate: "Qubit Quantum Mechanics with Correlated-Photon Experiments"

Matrix Based Formalism to Model Some Classic QM Experiments, Paper by Galvez, AJP 78, 510-519 (2010)

This document uses the Mathcad programming environment to model and reproduce most of the results for the experiments presented in Professor Galvez's paper.

Optical components such as mirrors,beam splitters, wave plates, and the entire interferometer can be represented by matrices. They perform the evolution of the state of the light as it propagates.

Polarization Space and Direction of Propagation: State Vectors

Photon moving horizontally: $x := \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

Photon moving vertically: $y := \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

Null vector: $n := \begin{pmatrix} 0 \\ 0 \end{pmatrix}$

Horizontal polarization: $h := \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

Vertical polarization: $v := \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

Diagonal polarization: $d := \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$

Single mode operators:

Projection operators for motion in the x- and y-directions: $X := \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$ $Y := \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$

Operator for polarizing film oriented at angle of θ to the horizontal.

$$\Theta_{op}(\theta) := \begin{pmatrix} \cos(\theta) \\ \sin(\theta) \end{pmatrix} \cdot (\cos(\theta) \quad \sin(\theta)) \rightarrow \begin{pmatrix} \cos(\theta)^2 & \cos(\theta)\cdot\sin(\theta) \\ \cos(\theta)\cdot\sin(\theta) & \sin(\theta)^2 \end{pmatrix}$$

Symmetric non-polarizing Beam Splitter, BS

Beam splitter: $BS := \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}$

Mirror: $M := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

Phase shift: $A(\delta) := \begin{pmatrix} e^{i\cdot\delta} & 0 \\ 0 & 1 \end{pmatrix}$

Half (W2) and quarter (W4) wave plates: $W_2 := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ $W_4 := \begin{pmatrix} 1 & 0 \\ 0 & -i \end{pmatrix}$

Identity: $I := \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

Rotated half wave plate: $W_2(\theta) := \begin{pmatrix} \cos(2\cdot\theta) & \sin(2\cdot\theta) \\ \sin(2\cdot\theta) & -\cos(2\cdot\theta) \end{pmatrix}$

Equation 17

$$W(\theta) := \begin{pmatrix} \cos(2\cdot\theta) & \sin(2\cdot\theta) & 0 & 0 \\ \sin(2\cdot\theta) & -\cos(2\cdot\theta) & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

Mach-Zehnder Interferometer, MZ:

$$MZ(\delta) := BS\cdot A(\delta)\cdot M\cdot BS$$

Two mode states and operators:

Single-photon direction of propagation and polarization states Eq 15:

$$xh := \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad xv := \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \quad yh := \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \quad yv := \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

Two-photon direction of propagation states.

$$xx := \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad xy := \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \quad yx := \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \quad yy := \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

Two-photon polarization states.

$$hh := \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad hv := \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \quad vh := \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \quad vv := \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

Polarizing Beam Splitter, PBS, which transmits horizontally polarized photons and reflects vertically polarized photons. Eq. 24

$$PBS := xh \cdot xh^T + yv \cdot xv^T + yh \cdot yh^T + xv \cdot yv^T \qquad PBS = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

Kronecker is Mathcad's command for tensor multiplication, ⊗, of square matrices.
kronecker(M, N) Multiplies matrix N by each element of matrix M,
returning an M•N by M•N array. Arguments: M and N are square matrices.

Polarization M-Z interferometer: $MZ_P(\delta) := PBS \cdot kronecker(A(\delta), I) \cdot kronecker(M, I) \cdot PBS$

Mathcad Simulation of MZI

Mach-Zehnder interferometer for direction of propagation and polarization, which places a rotatable half-wave plate in the upper path. Eq. 24

$$MZ_{dp}(\theta, \delta) := kronecker(BS, I) \cdot kronecker(A(\delta), I) \cdot W(\theta) \cdot kronecker(M, I) \cdot kronecker(BS, I)$$

Mach-Zehnder two-photon direction-of-propagation interferometer.

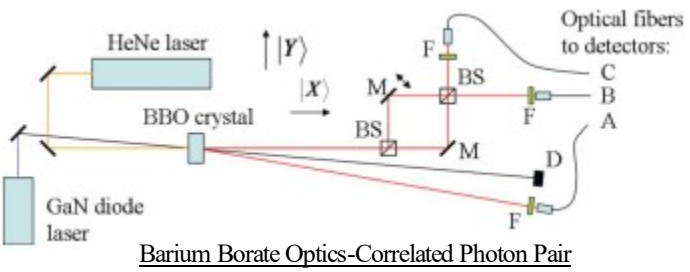
$$AA(\delta) := kronecker(A(\delta), A(\delta))$$

$$BSBS := kronecker(BS, BS) \quad MM := kronecker(M, M)$$

$$MZ_{dd}(\delta) := BSBS \cdot AA(\delta) \cdot MM \cdot BSBS$$

The results of Single Photons going through the interferometer and being detected at the two outputs of the interferometer are shown in Fig. 2.

Confirm the results in Figure 2 for the Mach-Zehnder interferometer:



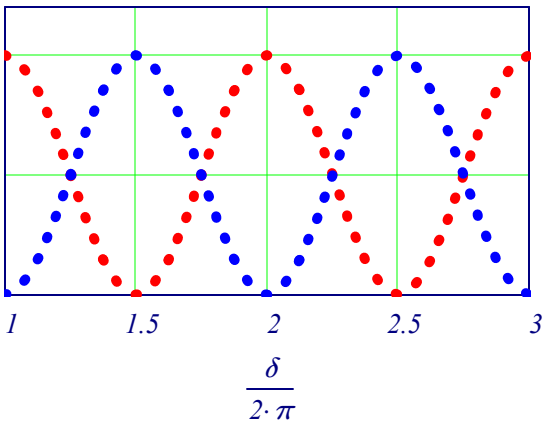
Barium Borate Optics-Correlated Photon Pair

Fig. 1. Standard layout for doing experiments with correlated photons. Interferometer components are **nonpolarizing beam splitters (BS)** and metallic mirrors (m). Band-pass filters (f) precede couplers to multimode fibers, which send light to detectors A, B, and C. The beam dump (d) collects the pump beam for safety.

$$\delta := 0, .125 \cdot \pi .. 6\pi$$

$$\left(\left|x^T \cdot MZ(\delta) \cdot x\right|\right)^2$$

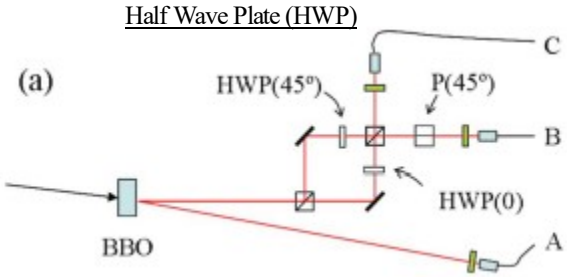
$$\left(\left|y^T \cdot MZ(\delta) \cdot x\right|\right)^2$$



Demonstrate that a superposition is formed after first beam splitter

$$BS \cdot x = \begin{pmatrix} 0.707 \\ 0.707i \end{pmatrix} \qquad \frac{1}{\sqrt{2}} \cdot (x + i \cdot y) = \begin{pmatrix} 0.707 \\ 0.707i \end{pmatrix}$$

$$\delta := 0, .1 \cdot \pi .. 2 \cdot \pi$$



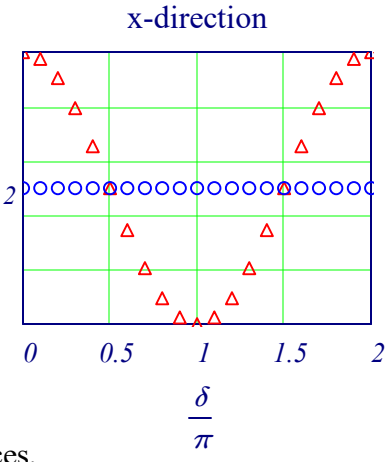
Barium Borate Optics-Correlated Photon Pair

Confirmation that path information destroys interference.

Fig. 3. Schematic of the (a) apparatus and (b) data for the quantum eraser. The data show cases when the light leaves the interferometer along the X direction not carrying path information (triangles) and when the light leaves along the Y direction carrying path information (circles) .

$\theta = 0$, no path information $\quad \left(\left| kronecker(X, I) \cdot MZ_{dp}(0, \delta) \cdot xv \right| \right)^2$

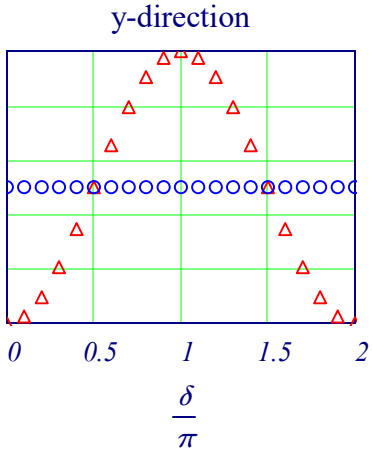
$\theta = \pi/4$, path information $\quad \left(\left| kronecker(X, I) \cdot MZ_{dp}\left(\frac{\pi}{4}, \delta\right) \cdot xv \right| \right)^2$



Kronecker is Mathcad's command for tensor multiplication of square matrices.

$\theta = 0$, no path information $\quad \left(\left| kronecker(Y, I) \cdot MZ_{dp}(0, \delta) \cdot xv \right| \right)^2$

$\theta = \pi/4$, path information $\quad \left(\left| kronecker(Y, I) \cdot MZ_{dp}\left(\frac{\pi}{4}, \delta\right) \cdot xv \right| \right)^2$



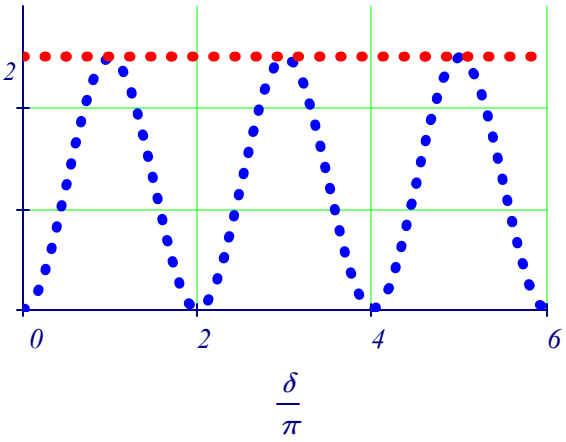
Erasure of path information restores interference. Erasers for the x- and y-directions place diagonal polarizers in those directions after the interferometer.

$$E_x := \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \qquad E_y := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} \end{pmatrix}$$

The x-direction has an eraser and the y-direction does not. $\delta := 0, .1 \cdot \pi .. 6\pi$

x-direction: $\left(\left| kronecker(X, I) \cdot E_x \cdot MZ_{dp}\left(\frac{\pi}{4}, \delta\right) \cdot xv \right| \right)^2$

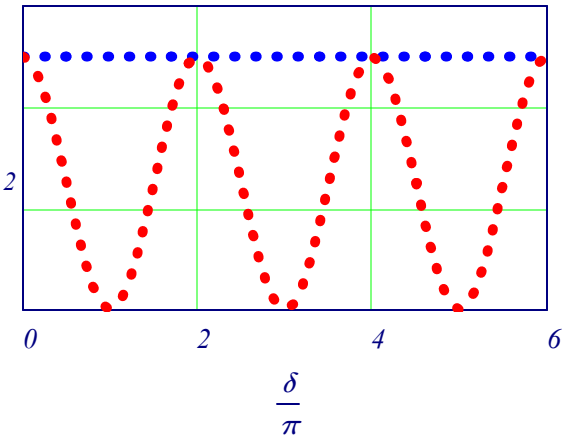
y-direction: $\left(\left| kronecker(Y, I) \cdot MZ_{dp}\left(\frac{\pi}{4}, \delta\right) \cdot xv \right| \right)^2$



The y-direction has an eraser and the x-direction does not.

x-direction: $\left(\left| kronecker(X, I) \cdot MZ_{dp}\left(\frac{\pi}{4}, \delta\right) \cdot xv \right| \right)^2$

y-direction: $\left(\left| kronecker(Y, I) \cdot E_y \cdot MZ_{dp}\left(\frac{\pi}{4}, \delta\right) \cdot xv \right| \right)^2$



For the MZ polarization interferometer diagonally polarized light enters in the x-direction, |xd>.
Tensor vector multiplication is awkward in Mathcad as is shown below.

$$\Psi_{in} := \frac{1}{\sqrt{2}} \cdot \begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

Note: Matrix indices begin at 0

$$submatrix(kronecker(augment(x, n), augment(d, n)), 0, 3, 0, 0) = \begin{pmatrix} 0.707 \\ 0.707 \\ 0 \\ 0 \end{pmatrix}$$

No light, however, exits in the x-direction. It exits in the y-direction showing no interference effects.

$\delta := 0, .2 \cdot \pi .. \pi$

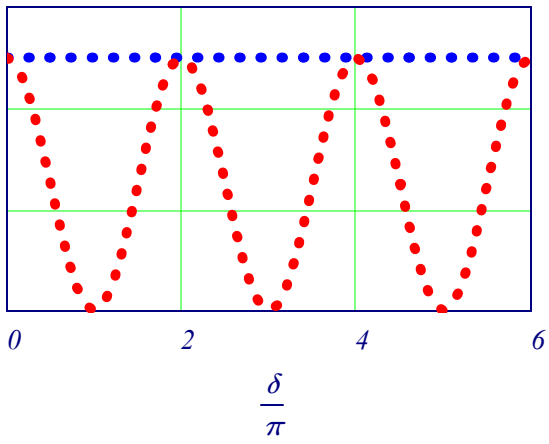
$$\left(\left| kronecker(X, I) \cdot MZ_P(\delta) \cdot \Psi_{in} \right| \right)^2 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \qquad \left(\left| kronecker(Y, I) \cdot MZ_P(\delta) \cdot \Psi_{in} \right| \right)^2 = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}$$

Placement of a **D** polarizer in the y-direction output erases distinguishing information and interference appears.

$\delta := 0, .1 \cdot \pi .. 6\pi$

x-direction: $\left(\left| kronecker(X, I) \cdot MZ_{dp}\left(\frac{\pi}{4}, \delta\right) \cdot xv \right| \right)^2$

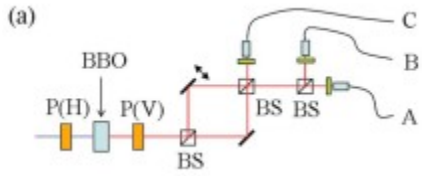
y-direction: $\left(\left| kronecker(Y, I) \cdot E_y \cdot MZ_{dp}\left(\frac{\pi}{4}, \delta\right) \cdot xv \right| \right)^2$



Calculation of exit probabilities for two photons in direction-of-propagation modes:

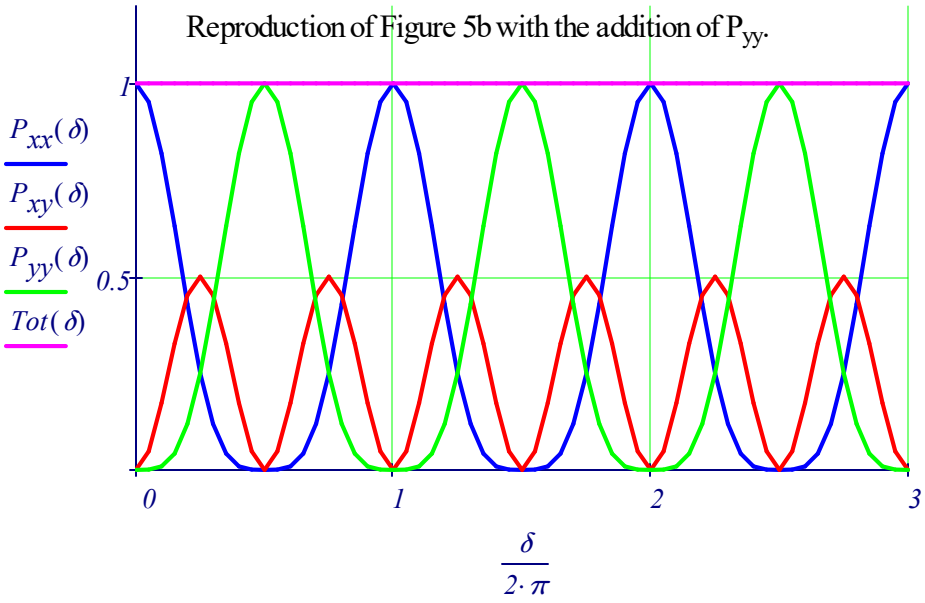
$$P_{xx}(\delta) := \left(\left| xx^T \cdot MZ_{dd}(\delta) \cdot xx \right| \right)^2 \qquad P_{xy}(\delta) := \left[\left| \frac{1}{\sqrt{2}} \cdot (xy + yx)^T \cdot MZ_{dd}(\delta) \cdot xx \right| \right]^2$$

$$P_{yy}(\delta) := \left(\left| yy^T \cdot MZ_{dd}(\delta) \cdot xx \right| \right)^2 \qquad Tot(\delta) := P_{xx}(\delta) + P_{xy}(\delta) + P_{yy}(\delta)$$



$\delta := 0, .05 \cdot \pi .. 6 \cdot \pi$

Reproduction of Figure 5b with the addition of P_{yy}.



"The striking result is that the (P_{xy}) interference pattern has twice the frequency of the single-photon interference pattern. Nonclassical interference shows new quantum aspects: two photons acting as a single quantum object (a biphoton)."

Hong-Ou-Mandel interference (right column, page 516):

$$BSBS \cdot \frac{1}{\sqrt{2}} \cdot (xy + yx) = \begin{pmatrix} 0.707i \\ 0 \\ 0 \\ 0.707i \end{pmatrix} \qquad \frac{i}{\sqrt{2}} \cdot (xx + yy) = \begin{pmatrix} 0.707i \\ 0 \\ 0 \\ 0.707i \end{pmatrix}$$

Section III.D deals with distinguishing between pure and mixed states experimentally. The pure state and it density matrix are given below.

$$\Psi_{pure} := \frac{1}{\sqrt{2}} \cdot (hh + vv) \qquad \Psi_{pure} = \begin{pmatrix} 0.707 \\ 0 \\ 0 \\ 0.707 \end{pmatrix} \qquad \Psi_{pure} \cdot \Psi_{pure}^{T} = \begin{pmatrix} 0.5 & 0 & 0 & 0.5 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0.5 & 0 & 0 & 0.5 \end{pmatrix}$$

The density matrix for the mixed state is calculated as follows.

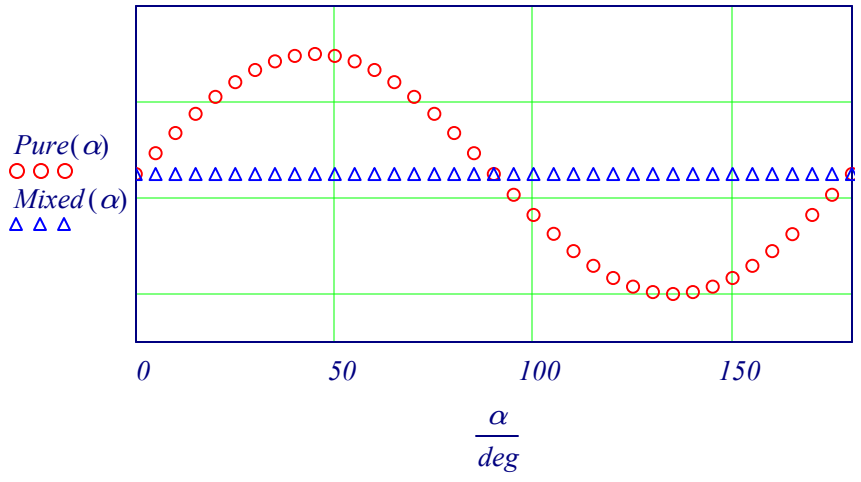
$$\frac{1}{2} \cdot hh \cdot hh^{T} + \frac{1}{2} \cdot vv \cdot vv^{T} = \begin{pmatrix} 0.5 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.5 \end{pmatrix}$$

The following calculations and their graphical representation are in complete agreement with section III.D

$$Pure(\alpha) := tr\left[\frac{1}{2} \cdot \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix} \cdot \frac{1}{2} \cdot \left[\begin{pmatrix} \cos(\alpha) \\ \cos(\alpha) \\ \sin(\alpha) \\ \sin(\alpha) \end{pmatrix} \cdot \begin{pmatrix} \cos(\alpha) \\ \cos(\alpha) \\ \sin(\alpha) \\ \sin(\alpha) \end{pmatrix}^{T} \right] \right] \text{ simplify } \rightarrow \frac{\sin(2 \cdot \alpha)}{4} + \frac{1}{4}$$

$$Mixed(\alpha) := tr\left[\frac{1}{2} \cdot \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \cdot \frac{1}{2} \cdot \left[\begin{pmatrix} \cos(\alpha) \\ \cos(\alpha) \\ \sin(\alpha) \\ \sin(\alpha) \end{pmatrix} \cdot \begin{pmatrix} \cos(\alpha) \\ \cos(\alpha) \\ \sin(\alpha) \\ \sin(\alpha) \end{pmatrix}^{T} \right] \right] \text{ simplify } \rightarrow \frac{1}{4}$$

Reproduce Figure 6 results. $\alpha := 0 \cdot deg, 5 \cdot deg .. 180 \cdot deg$



The following calculation are in agreement with the math in the final paragraph of section IV.D.

$$kronecker\left(W_2(0), I\right) \cdot \Psi_{pure} = \begin{pmatrix} 0.707 \\ 0 \\ 0 \\ -0.707 \end{pmatrix} \begin{pmatrix} 0.707 \\ 0 \\ 0 \\ -0.707 \end{pmatrix} \cdot \begin{pmatrix} 0.707 \\ 0 \\ 0 \\ -0.707 \end{pmatrix}^T = \begin{pmatrix} 0.5 & 0 & 0 & -0.5 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -0.5 & 0 & 0 & 0.5 \end{pmatrix}$$

$$kronecker\left(W_2(0), I\right) \cdot \Psi_{pure} \cdot \Psi_{pure}^{\ T} \cdot kronecker\left(W_2(0), I\right)^T = \begin{pmatrix} 0.5 & 0 & 0 & -0.5 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -0.5 & 0 & 0 & 0.5 \end{pmatrix}$$

$$Pure(\alpha) := tr\left[\frac{1}{2} \cdot \begin{pmatrix} 1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 1 \end{pmatrix} \cdot \frac{1}{2} \cdot \left[\begin{pmatrix} \cos(\alpha) \\ \cos(\alpha) \\ \sin(\alpha) \\ \sin(\alpha) \end{pmatrix} \cdot \begin{pmatrix} \cos(\alpha) \\ \cos(\alpha) \\ \sin(\alpha) \\ \sin(\alpha) \end{pmatrix}^T\right]\right] \text{ simplify } \rightarrow \frac{1}{4} - \frac{\sin(2 \cdot \alpha)}{4}$$

The Galvez paper shows this as [1 - sin(α)]/4, which is a typographical error. The correct answer is [1 - sin(2*α)]/4

XVIII. Simple Simulation of Parallel Quantum Computation

This tutorial deals with quantum function evaluation and parallel computation. The example is taken from pages 94-95 of *Exploring the Quantum* by Haroche and Raimond. A certain function of x yields the following table of results.

Computing a function f(x) with a quantum machine

$$\begin{pmatrix} x & 0 & 1 \\ f(x) & 1 & 0 \end{pmatrix}$$

First we establish that the **circuit shown below** yields the results given in the table, and then demonstrate that it also **carries out a parallel calculation** in one step using both input values of x.

Exclusive OR = $\oplus$

where, for example $|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ $|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

The top wire carries the value of x and the bottom wire is initially set to |0>. After operation of the controlled-NOT and NOT gates, x remains on the top wire while the bottom wire carries the value of the function, f(x). In other words,

$$\hat{U}_f|x\rangle|0\rangle = |x\rangle|f(x)\rangle$$

CNOT can be Represented by Pauli Basis:

$$\text{CNOT} = e^{i\frac{\pi}{4}(I-Z_1)(I-X_2)}$$

The action of the CNOT gate can also be represented by the matrix (permutation matrix form: one entry of 1 in each row:)

The quantum gates in matrix form are: $I := \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ $NOT := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ $CNOT := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$

U_f(controlled-NOT, followed by a NOT operation on the lower wire) is a reversible operator. Doing it twice in succession on the initial two-qubit state is equivalent to the identity operation.
Note that the identity operator is required when a wire is not involved in an operation. In what follows the quantum circuit is constructed, displayed and its reversibility demonstrated. In other words, repeating the circuit is equivalent to the identity operation. Reversibility is a crucial property in quantum computer circuitry.

Kronecker is Mathcad's command for carrying out matrix tensor multiplication.

$$QuantumCircuit := kronecker(I, NOT) \cdot CNOT$$

$$QuantumCircuit = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \qquad QuantumCircuit^2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Given the simplicity of the matrix representing the circuit, the following calculations can easily be done by hand.

	Input	Calculation	Output
f(0) = 1	$\begin{pmatrix}1\\0\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix}=\begin{pmatrix}1\\0\\0\\0\end{pmatrix}$	$QuantumCircuit\cdot\begin{pmatrix}1\\0\\0\\0\end{pmatrix}=\begin{pmatrix}0\\1\\0\\0\end{pmatrix}$	$\begin{pmatrix}0\\1\\0\\0\end{pmatrix}=\begin{pmatrix}1\\0\end{pmatrix}\otimes\begin{pmatrix}0\\1\end{pmatrix}$
f(1) = 0	$\begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix}=\begin{pmatrix}0\\0\\1\\0\end{pmatrix}$	$QuantumCircuit\cdot\begin{pmatrix}0\\0\\1\\0\end{pmatrix}=\begin{pmatrix}0\\0\\1\\0\end{pmatrix}$	$\begin{pmatrix}0\\0\\1\\0\end{pmatrix}=\begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix}$

These calculations demonstrate that **the quantum circuit is a valid algorithm for the calculation of f(x)**. We now demonstrate parallel computation by putting |x> in a balanced superposition of |0> and |1>. As shown below, the operation of the circuit yields a superposition of the previous results. The function has been evaluated for both values of x in a single pass through the circuit.

$$\frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix}=\frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\1\\0\end{pmatrix}\qquad QuantumCircuit\cdot\frac{1}{\sqrt{2}}\cdot\begin{pmatrix}1\\0\\1\\0\end{pmatrix}=\begin{pmatrix}0\\0.707\\0.707\\0\end{pmatrix}$$

$$\frac{1}{\sqrt{2}}\cdot\begin{pmatrix}0\\1\\1\\0\end{pmatrix}=\frac{1}{\sqrt{2}}\cdot\left[\begin{pmatrix}0\\1\\0\\0\end{pmatrix}+\begin{pmatrix}0\\0\\1\\0\end{pmatrix}\right]=\frac{1}{\sqrt{2}}\cdot\left[\begin{pmatrix}1\\0\end{pmatrix}\cdot\begin{pmatrix}0\\1\end{pmatrix}+\begin{pmatrix}0\\1\end{pmatrix}\cdot\begin{pmatrix}1\\0\end{pmatrix}\right]$$

Haroche and Raimond describe this process as follows: "By superposing the inputs of a computation, one operates the machine 'in parallel', **making it compute simultaneously all the values of a function** and keeping its state, before any final bit detection is performed, s**uspended in a coherent superposition of all the possible outcome**s." In summary, simple calculations have demonstrated how a quantum circuit can function as an algorithm for the evaluation of a mathematical function, and how the same circuit is capable of parallel evaluations of that function.

Input	Operation	Intermediate	Operation	Output
$\lvert 00\rangle$		$\lvert 00\rangle$		$\lvert 01\rangle$
$\lvert 10\rangle$	$\xrightarrow{\text{CNOT}}$	$\lvert 11\rangle$	$\xrightarrow{1\otimes\text{NOT}}$	$\lvert 10\rangle$
$\frac{1}{\sqrt{2}}\left[\lvert 0\rangle+\lvert 1\rangle\right]\lvert 0\rangle=\frac{1}{\sqrt{2}}\left[\lvert 00\rangle+\lvert 10\rangle\right]$		$\frac{1}{\sqrt{2}}\left[\lvert 00\rangle+\lvert 11\rangle\right]$		$\frac{1}{\sqrt{2}}\left[\lvert 01\rangle+\lvert 10\rangle\right]$

However, as Haroche and Raimond note, on a practical level only one result can be realized for each operation of the circuit because on measurement the superposition created by the circuit collapses to one of the states forming the superposition. This is simulated with projection operators (|0><0| and |1><1|) on both registers for the four possible measurement outcomes for each value of x.

$$f(0) = 0 \qquad \left[kronecker\left[\begin{pmatrix} 1 \\ 0 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix}^T , \begin{pmatrix} 1 \\ 0 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix}^T \right] \cdot QuantumCircuit \cdot \frac{1}{\sqrt{2}} \cdot \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix} \right]^2 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

$$f(0) = 1 \qquad \left[kronecker\left[\begin{pmatrix} 1 \\ 0 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix}^T , \begin{pmatrix} 0 \\ 1 \end{pmatrix} \cdot \begin{pmatrix} 0 \\ 1 \end{pmatrix}^T \right] \cdot QuantumCircuit \cdot \frac{1}{\sqrt{2}} \cdot \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix} \right]^2 = \begin{pmatrix} 0 \\ 0.5 \\ 0 \\ 0 \end{pmatrix}$$

$$f(1) = 0 \qquad \left[kronecker\left[\begin{pmatrix} 0 \\ 1 \end{pmatrix} \cdot \begin{pmatrix} 0 \\ 1 \end{pmatrix}^T , \begin{pmatrix} 1 \\ 0 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix}^T \right] \cdot QuantumCircuit \cdot \frac{1}{\sqrt{2}} \cdot \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix} \right]^2 = \begin{pmatrix} 0 \\ 0 \\ 0.5 \\ 0 \end{pmatrix}$$

$$f(1) = 1 \qquad \left[kronecker\left[\begin{pmatrix} 0 \\ 1 \end{pmatrix} \cdot \begin{pmatrix} 0 \\ 1 \end{pmatrix}^T , \begin{pmatrix} 0 \\ 1 \end{pmatrix} \cdot \begin{pmatrix} 0 \\ 1 \end{pmatrix}^T \right] \cdot QuantumCircuit \cdot \frac{1}{\sqrt{2}} \cdot \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix} \right]^2 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

As Haroche and Raimond write, "It is, however, one thing to compute potentially at once all the values of f(x) and quite another to be able to exploit this quantum parallelism and extract from it more information than from a mundane classical computation. The final stage of information acquisition must always be a measurement." Therefore, the exploitation of quantum parallelism for practical purposes such as searches and factorization requires more elaborate quantum circuits than the one presented here.

Truth tables for quantum circuit elements:

Identity

0	to	0
1	to	1

NOT

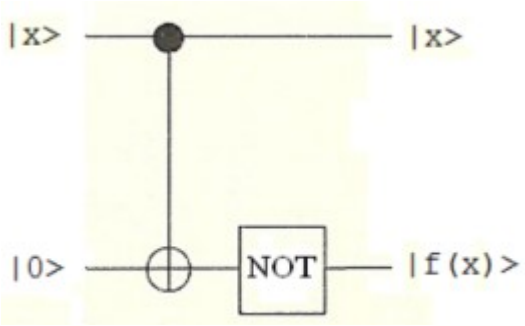
0	to	1
1	to	0

CNOT

Decimal	Binary	to	Binary	Decimal
0	00	to	00	0
1	01	to	01	1
2	10	to	11	3
3	11	to	10	2

XIX. Simulation of the Deutsch-Jozsa Algorithm

The D-J Algorithm demonstrates that there is a problem for which a QC runs faster than a Classic Computer.
Specifically, given a boolean function whose input is 1 bit f: : {0,1} --> {0,1}, is it constant?
The following circuit produces the table of results to its right. The top wires carry the value of x and the circuit places f(x) on the bottom wire. As is shown in the previous Section (XII), this circuit can also operate in parallel accepting as input all x-values and returning on the bottom wire a superposition of all values of f(x).



$$\begin{pmatrix} x & 0 & 1 & 2 & 3 \\ f(x) & 1 & 0 & 0 & 1 \end{pmatrix}$$ where

|0> = |0>|0>

|1> = |0>|1>

|2> = |1>|0>

|3> = |1>|1>

The function belongs to the balanced category because it produces 0 and 1 with equal frequency. A modification of this circuit (Ith algorithm, p.298 in *The Quest for the Quantum Computer*, by Julian Brown) answers the question of whether the function is constant or balanced. Naturally we already know the answer, so this is a simple demonstration that the circuit works.

The input is **|0>|0>|1>** followed by a Hadamard gate on each wire, as shown in the circuit shown below. As is well known the Hadamard operation creates the following superposition states.

$$H\cdot\begin{pmatrix}1\\0\end{pmatrix} = \frac{1}{\sqrt{2}}\cdot\begin{pmatrix}1\\1\end{pmatrix} \qquad H\cdot\begin{pmatrix}0\\1\end{pmatrix} = \frac{1}{\sqrt{2}}\cdot\begin{pmatrix}1\\-1\end{pmatrix}$$

Therefore the Hadamard operation transforms the input state to the following three-qubit state which is fed to the quantum circuit.

$$\frac{1}{\sqrt{2}}\cdot\begin{pmatrix}1\\1\end{pmatrix}\cdot\frac{1}{\sqrt{2}}\cdot\begin{pmatrix}1\\1\end{pmatrix}\cdot\frac{1}{\sqrt{2}}\cdot\begin{pmatrix}1\\-1\end{pmatrix} = \frac{1}{2\cdot\sqrt{2}}\cdot\begin{pmatrix}1\\-1\\1\\-1\\1\\-1\\1\\-1\end{pmatrix}$$

The following matrices are required to execute the circuit. $I := \begin{pmatrix}1&0\\0&1\end{pmatrix}$ $NOT := \begin{pmatrix}0&1\\1&0\end{pmatrix}$ $H := \frac{1}{\sqrt{2}}\cdot\begin{pmatrix}1&1\\1&-1\end{pmatrix}$

$$CNOT := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \quad CnNOT := \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

After the portion of the quantum circuit shown above, Hadamard gates are added to the top two wires, as shown in the circuit on 2nd page down. The matrix representing the circuit is assembled using tensor matrix multiplication and then allowed to operate on the wave function. The full circuit is shown below.

$$QCkt := kronecker(H, kronecker(H, I)) \cdot kronecker(I, kronecker(I, NOT)) \cdot kronecker(I, CNOT) \cdot CnNOT$$

$$QCkt = \frac{1}{2} \cdot \begin{pmatrix} 0 & 1 & 1 & 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 & 1 & 1 & 0 \\ 0 & 1 & -1 & 0 & 1 & 0 & 0 & -1 \\ 1 & 0 & 0 & -1 & 0 & 1 & -1 & 0 \\ 0 & 1 & 1 & 0 & -1 & 0 & 0 & -1 \\ 1 & 0 & 0 & 1 & 0 & -1 & -1 & 0 \\ 0 & 1 & -1 & 0 & -1 & 0 & 0 & 1 \\ 1 & 0 & 0 & -1 & 0 & -1 & 1 & 0 \end{pmatrix} \quad QCkt \cdot \frac{1}{2 \cdot \sqrt{2}} \cdot \begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \\ 1 \\ -1 \\ 1 \\ -1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ -0.707 \\ 0.707 \end{pmatrix} \quad \begin{pmatrix} 0 \\ 1 \end{pmatrix} \cdot \begin{pmatrix} 0 \\ 1 \end{pmatrix} \cdot \frac{1}{\sqrt{2}} \cdot \begin{pmatrix} -1 \\ 1 \end{pmatrix}$$

Next the qubits on the top two wires are measured. If both are |0> the function is constant, but if at least one is **|1>** the function is balanced. The measurement on the top wires is implemented with projection operators **|0><0|** and **|1><1|,** and confirms that the function is not constant but belongs to the balanced category.

The first qubit is not |0>.

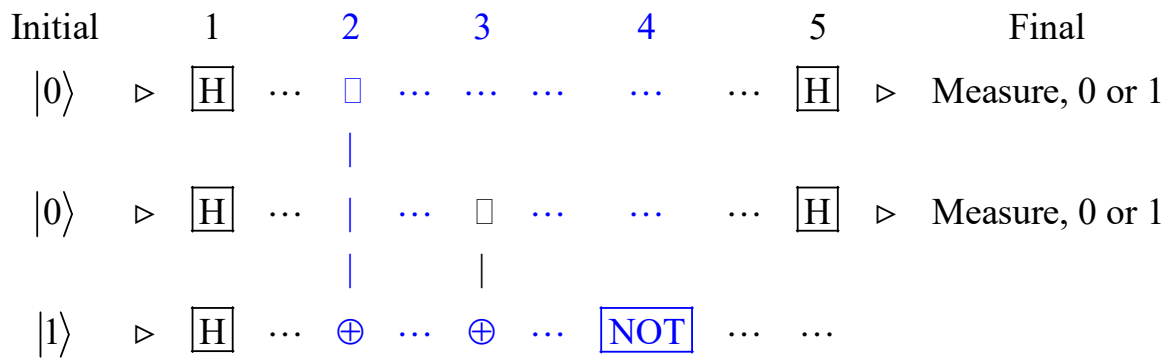
$$kronecker\left[\begin{pmatrix} 1 \\ 0 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix}^T, kronecker(I, I)\right] \cdot QCkt \cdot \frac{1}{2 \cdot \sqrt{2}} \cdot \begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \\ 1 \\ -1 \\ 1 \\ -1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

The second qubit is not |0>. $kronecker\left[I, kronecker\left[\begin{pmatrix}1\\0\end{pmatrix}\cdot\begin{pmatrix}1\\0\end{pmatrix}^{T}, I\right]\right]\cdot QCkt\cdot\frac{1}{2\cdot\sqrt{2}}\cdot\begin{pmatrix}1\\-1\\1\\-1\\1\\-1\\1\\-1\end{pmatrix}=\begin{pmatrix}0\\0\\0\\0\\0\\0\\0\\0\end{pmatrix}$

The first qubit is **|1>.** $kronecker\left[\begin{pmatrix}0\\1\end{pmatrix}\cdot\begin{pmatrix}0\\1\end{pmatrix}^{T}, kronecker(I, I)\right]\cdot QCkt\cdot\frac{1}{2\cdot\sqrt{2}}\cdot\begin{pmatrix}1\\-1\\1\\-1\\1\\-1\\1\\-1\end{pmatrix}=\begin{pmatrix}0\\0\\0\\0\\0\\0\\-0.707\\0.707\end{pmatrix}$

The second qubit is **|1>.** $kronecker\left[I, kronecker\left[\begin{pmatrix}0\\1\end{pmatrix}\cdot\begin{pmatrix}0\\1\end{pmatrix}^{T}, I\right]\right]\cdot QCkt\cdot\frac{1}{2\cdot\sqrt{2}}\cdot\begin{pmatrix}1\\-1\\1\\-1\\1\\-1\\1\\-1\end{pmatrix}=\begin{pmatrix}0\\0\\0\\0\\0\\0\\-0.707\\0.707\end{pmatrix}$

The following illustrates an algebraic analysis of the Deutsch-Jozsa algorithm.



$$H|0\rangle \to \frac{1}{\sqrt{2}}\left[|0\rangle + |1\rangle\right] \qquad H|1\rangle \to \frac{1}{\sqrt{2}}\left[|0\rangle - |1\rangle\right]$$

NOT

$$\begin{pmatrix} 0 & ' & 1 \\ 1 & ' & 0 \end{pmatrix}$$

CNO

$$\begin{pmatrix} \text{Decimal} & \text{Binary} & ' & \text{Binary} & \text{Decimal} \\ 0 & 00 & ' & 00 & 0 \\ 1 & 01 & ' & 01 & 1 \\ 2 & 10 & ' & 11 & 3 \\ 3 & 11 & ' & 10 & 2 \end{pmatrix}$$

CnNO

$$\begin{pmatrix} \text{Decimal} & \text{Binary} & ' & \text{Binary} & \text{Decimal} \\ 0 & 000 & ' & 000 & 0 \\ 1 & 001 & ' & 001 & 1 \\ 2 & 010 & ' & 010 & 2 \\ 3 & 011 & ' & 011 & 3 \\ 4 & 100 & ' & 101 & 5 \\ 5 & 101 & ' & 100 & 4 \\ 6 & 110 & ' & 111 & 7 \\ 7 & 111 & ' & 110 & 6 \end{pmatrix}$$

$$|001\rangle$$

$$H \otimes H \otimes H$$

$$\frac{1}{\sqrt{2}}\left[|0\rangle+|1\rangle\right]\frac{1}{\sqrt{2}}\left[|0\rangle+|1\rangle\right]\frac{1}{\sqrt{2}}\left[|0\rangle-|1\rangle\right]=\frac{1}{2\sqrt{2}}\left[|000\rangle-|001\rangle+|010\rangle-|011\rangle+|100\rangle-|101\rangle+|110\rangle-|111\rangle\right]$$

CnNOT

$$\frac{1}{2\sqrt{2}}\left[|000\rangle-|001\rangle+|010\rangle-|011\rangle+|101\rangle-|100\rangle+|111\rangle-|110\rangle\right]$$

$$I \otimes CNOT$$

$$\frac{1}{2\sqrt{2}}\left[|000\rangle-|001\rangle+|011\rangle-|010\rangle+|101\rangle-|100\rangle+|110\rangle-|111\rangle\right]$$

$$I \otimes I \otimes NOT$$

$$\frac{1}{\sqrt{2}}\left[|0\rangle-|1\rangle\right]\frac{1}{\sqrt{2}}\left[|0\rangle-|1\rangle\right]\frac{1}{\sqrt{2}}\left[|1\rangle-|0\rangle\right]$$

$$H \otimes H \otimes I$$

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

Since the top wires contain $|\mathbf{1}>$, the function is balanced. **This algorithm illustrates the roles of superposition, entanglement and interference in quantum computation**. Regarding the latter, it is destructive interference in the last step that eliminates unwanted outcomes yielding the final result on the last line.

One pass through the quantum circuit answers the question (is the function balanced or constrant) that would take 4 calculations on a classical computer. Thus given this problem, a QC is faster than a classical computer.

The interference that occurs in the last step is illustrated by letting |a>=|0> and |b>=|1> and carrying out Hadamard transforms on the first two qubits.

$$\frac{1}{4\cdot\sqrt{2}}\cdot\begin{bmatrix}\left(a_1+b_1\right)\cdot\left(a_2+b_2\right)\cdot b_3-\left(a_1+b_1\right)\cdot\left(a_2+b_2\right)\cdot a_3\ \ldots\\ +\left(a_1+b_1\right)\cdot\left(a_2-b_2\right)\cdot b_3-\left(a_1+b_1\right)\cdot\left(a_2-b_2\right)\cdot a_3\ \ldots\\ +\left(a_1-b_1\right)\cdot\left(a_2+b_2\right)\cdot b_3-\left(a_1-b_1\right)\cdot\left(a_2+b_2\right)\cdot a_3\ \ldots\\ +\left(a_1-b_1\right)\cdot\left(a_2-b_2\right)\cdot b_3-\left(a_1-b_1\right)\cdot\left(a_2-b_2\right)\cdot a_3\end{bmatrix}\ \text{simplify}\ \rightarrow -\frac{\sqrt{2}\cdot a_1\cdot a_2\cdot\left(a_3-b_3\right)}{2}$$

XX. Quantum Restrictions on Cloning

Tutorial: *Quantum communication with photons,* Mario Krenn, https://arxiv.org/pdf/1701.00989.pdf

The Quantum Bit

In classical information and computation science, information is encoded in the most fundamental entity, the bit. Its two possible values 0 and 1 are physically realized in many ways, be it simply by mechanical means (as a switch), in solids by magnetic or ferroelectric domains (hard drives), or by light pulses (optical digital media). All of these methods have one thing in common—one state of the device mutually excludes the simultaneous presence of the other—the switch is **either on or off**.

The superposition principle entails one of the **most fundamental aspects of quantum physics**, namely to allow the description of a physical system as being in a **probabilistic combination of its alternative states**. This so-called Superposition of states not only provides all predictions for the outcome of physical measurement, it also has drastic consequences for the nature of the physical state that we ascribe to a system. Its most important direct implication is the so-called **no-cloning theorem**, which states that it is **impossible to obtain a perfect copy of a qubit in an unknown state without destroying the information content of the original**. The no-cloning theorem is the basis for the security of all quantum communication schemes described in the following sections.

To fully understand a qubit, it is important to distinguish between a coherent superposition and a mixture of possible states. For its use in quantum communication, it is important that a photon exists in a coherent superposition of its **possible states**. For example, a polarization qubit being in a coherent superposition of horizontal and vertical polarizations (with a certain phase relation) can be understood as a photon polarized diagonally at +45◦. A polarizer set at this angle will **always transmit such a photon with 100% probability** (and zero probability when set to −45◦). However, a photon in a **mixture (incoherent** superposition) of horizontal and vertical polarization states will be **transmitted with 50% probability**. **Quantum superpositions,** however, are **not limited to just two possible states.** The information carried by a photon is **potentially enormous**. While **polarization is necessarily a two-level (qubit) property,** other degrees of freedom of a photon such as its spatial or temporal structure can have many orthogonal levels. For example, a photon can exist in a coherent superposition of different paths coming out of a multi-port beam splitter. These types of superpositions are referred to as "**high-dimensional**" by virtue of their ability to **encode large amounts of information**.

Practical Introduction to Quantum Computing: From Qubits to Quantum Machine Learning, CERN

- The way to know the value of a qubit is to perform a measurement. However
- The result of the measurement is random
- When we measure, we only obtain one (classical) bit of information
- If we measure the state $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ we get 0 with probability $|\alpha|^2$ and 1 with probability $|\beta|^2$
- Moreover, the new state after the measurement will be $|0\rangle$ or $|1\rangle$ depending of the result we have obtained (wavefunction collapse)
- We cannot perform several independent measurements of $|\psi\rangle$ because we cannot copy the state (no-cloning theorem)

No Cloning Matrix Proof

Tutorial: *Physical_and_Theoretical_Chemistry,* Dr. Frank Rioux

Suppose a quantum copier exists which is able to carry out the following cloning operation.

$$\begin{pmatrix}0\\1\end{pmatrix} \xrightarrow{\text{Clone}} \begin{pmatrix}0\\1\end{pmatrix} \otimes \begin{pmatrix}0\\1\end{pmatrix} = \begin{pmatrix}0\\0\\0\\1\end{pmatrix}$$

Next the cloning operation (using the same copier) is carried out on the **general qubit** shown below.

$$\begin{pmatrix}\cos(\theta)\\ \sin(\theta)\end{pmatrix}\xrightarrow{\text{Clone}}\begin{pmatrix}\cos(\theta)\\ \sin(\theta)\end{pmatrix}\otimes\begin{pmatrix}\cos(\theta)\\ \sin(\theta)\end{pmatrix}=\begin{pmatrix}\cos^2(\theta)\\ \cos(\theta)\sin(\theta)\\ \sin(\theta)\cos(\theta)\\ \sin^2(\theta)\end{pmatrix}$$

Quantum transformations are unitary, meaning probability is preserved. This requires that the scalar products of the initial and final states must be the same.

$$\text{Initial state:}\quad \begin{pmatrix}\cos(\theta) & \sin(\theta)\end{pmatrix}\begin{pmatrix}0\\ 1\end{pmatrix}=\sin(\theta)$$

$$\text{Final state:}\quad \begin{pmatrix}\cos^2(\theta) & \cos(\theta)\sin(\theta) & \sin(\theta)\cos(\theta) & \sin^2(\theta)\end{pmatrix}\begin{pmatrix}0\\ 0\\ 0\\ 1\end{pmatrix}=\sin^2(\theta)$$

It is clear from this analysis that quantum theory puts a significant restriction on copying.
Only states for which sin(θ) = 0 or 1 (0 and 90 degrees) can be copied by the original clone.

In conclusion, two quotes from Otters and Azure, *Physics Today*, February 2009, page 76.

Perfect copying can be achieved only when the two states are orthogonal, and even then one can copy those two states (...) only with a copier specifically built for that set of states.
In sum, one cannot make a perfect copy of an unknown quantum state, since, without prior knowledge, it is impossible to select the right copier for the job. That formulation is one common way of stating the no-cloning theorem.

An equivalent way to look at this (**See:** ***Quantum communication with photons***, Mario Krenn) , Page 8
Assume that a clone exists for the V-H polarization states.

$$\hat{C}|V\rangle|X\rangle=|V\rangle|V\rangle \qquad \hat{C}|H\rangle|X\rangle=|H\rangle|H\rangle$$ Equations 1 and 2.

A diagonally polarized photon is a superposition of the V-H polarization states.

$$|D\rangle=\frac{1}{\sqrt{2}}\left(|V\rangle+|H\rangle\right)$$

However, due to the linearity of quantum mechanics **the V-H clone cannot clone a diagonally polarized photon.**

$$\hat{C}|D\rangle|X\rangle=\hat{C}\frac{1}{\sqrt{2}}\left(|V\rangle+|H\rangle\right)|X\rangle=\frac{1}{\sqrt{2}}\left(\hat{C}|V\rangle|X\rangle+\hat{C}|H\rangle|X\rangle\right)=\frac{1}{\sqrt{2}}\left(|V\rangle|V\rangle+|H\rangle|H\rangle\right)$$

$$\hat{C}|D\rangle|X\rangle\neq|D\rangle|D\rangle=\frac{1}{2}\left(|V\rangle|V\rangle+|V\rangle|H\rangle+|H\rangle|V\rangle+|H\rangle|H\rangle\right)$$ Equation 3

The last line in equation (3) was obtained by using equations (1) and (2) for the cloning operator ˆC. The result is an entangled state that cannot be factorized into |DA> |DA>. If one were to measure either of the entangled photons individually, the result would be random, and certainly not |DA>. From this simple example it's clear that quantum cloning is not possible.

XXII. Factoring Using Shor's Quantum Algorithm

Quantum Computation, by David P. DiVincenzo, *Physical_and_Theoretical_Chemistry*, Dr. Frank Rioux

This tutorial presents a toy calculation dealing with the quantum factorization of 15 using Shor's algorithm. The first step is to find the period of $\mathbf{a^x}$ **modulo 15**, where **a** is chosen randomly.

$$a := 4 \qquad N := 15 \qquad f(x) := mod\left(a^x, N\right) \qquad Q := 4 \qquad x := 0..Q-1 \qquad x = \begin{pmatrix} 0 \\ 1 \\ 2 \\ 3 \end{pmatrix} \qquad f(x) = \begin{pmatrix} 1 \\ 4 \\ 1 \\ 4 \end{pmatrix}$$

We proceed by ignoring the fact that we can see by inspection that the period of f(x) is 2 and demonstrate how it is determined using a quantum (discrete) Fourier transform. After the registers are loaded with x and f(x) using a **quantum** computer, they exist in the following **superposition**.

$$\frac{1}{\sqrt{Q}}\sum_{x=0}^{Q-1}|x\rangle|f(x)\rangle = \frac{1}{2}\left[|0\rangle|1\rangle + |1\rangle|4\rangle + |2\rangle|1\rangle + |3\rangle|4\rangle + \cdots\right]$$

The next step is to find the period of f(x) by performing a quantum Fourier transform (QFT) on the input register **|x>**.

$$Q := 4 \qquad mm := 0..Q-1 \qquad n := 0..Q-1 \qquad QFT_{mm,n} := \frac{1}{\sqrt{Q}}\cdot exp\left(i\cdot\frac{2\cdot\pi\cdot mm\cdot n}{Q}\right)$$

$$QFT = \begin{pmatrix} 0.5 & 0.5 & 0.5 & 0.5 \\ 0.5 & 0.5i & -0.5 & -0.5i \\ 0.5 & -0.5 & 0.5 & -0.5 \\ 0.5 & -0.5i & -0.5 & 0.5i \end{pmatrix}$$

$x = 0 \qquad QFT\cdot\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0.5 \\ 0.5 \\ 0.5 \\ 0.5 \end{pmatrix}$

$x = 1 \qquad QFT\cdot\begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0.5 \\ 0.5i \\ -0.5 \\ -0.5i \end{pmatrix}$

$x = 2 \qquad QFT\cdot\begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0.5 \\ -0.5 \\ 0.5 \\ -0.5 \end{pmatrix}$

$x = 3 \qquad QFT\cdot\begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0.5 \\ -0.5i \\ -0.5 \\ 0.5i \end{pmatrix}$

The operation of the QFT on the x-register is expressed algebraically in the middle term below.
Quantum interference in this term yields the result on the right which **shows a period of 2 on the x-register.**

$$QFT(x)\frac{1}{2}\left[|0\rangle|1\rangle + |1\rangle|4\rangle + |2\rangle|1\rangle + |3\rangle|4\rangle\right] = \begin{aligned} &\frac{1}{4}\left[|0\rangle + |1\rangle + |2\rangle + |3\rangle\right]|1\rangle \\ &+\frac{1}{4}\left[|0\rangle + i|1\rangle - |2\rangle - i|3\rangle\right]|4\rangle \\ &+\frac{1}{4}\left[|0\rangle - |1\rangle + |2\rangle - |3\rangle\right]|1\rangle \\ &+\frac{1}{4}\left[|0\rangle - i|1\rangle - |2\rangle + i|3\rangle\right]|4\rangle \end{aligned} = \frac{1}{2}\left[|0\rangle\left(|1\rangle + |4\rangle\right) + |2\rangle\left(|1\rangle - |4\rangle\right)\right]$$

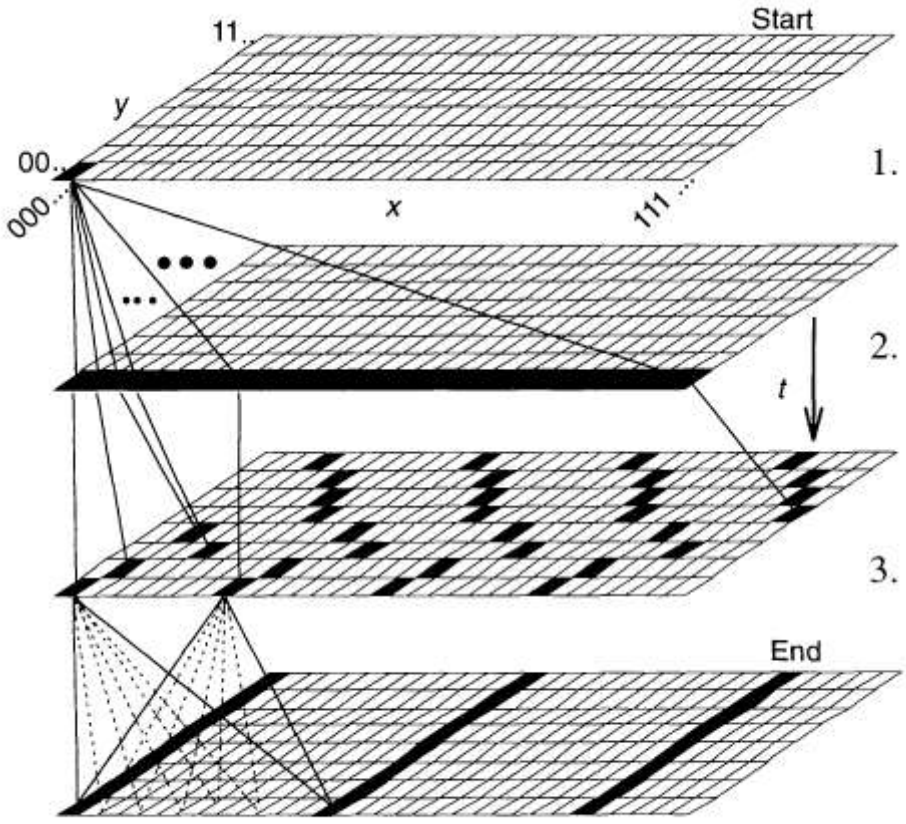
The next step is to use the Euclidian algorithm by calculating the greatest common divisor of two functions involving the period and **a**, and the number to be factored, **N**. This yields the prime factors of 15.

$$period := 2 \qquad gcd\left(a^{\frac{period}{2}} - 1, N\right) = 3 \qquad gcd\left(a^{\frac{period}{2}} + 1, N\right) = 5$$

Figure 5 (Shown Below) in "*Quantum Computation*," by David P. DiVincenzo, *Science* **270**, 258 (1995) provides a succinct graphical illustration of the steps of Shor's factorization algorithm.

> A schematic depiction of the time evolution pathways in Shor's prime factoring procedure. The computational states appearing in the wave function at each selected instant in time are indicated by the filled rectangles. A few of the pathways are sketched out. Most of the pathways in the final step (dotted lines) interfere destructively, with only a few (solid lines) interfering constructively.

The shading in the Figure indicates the instantaneous state vector throughout the three main stages of Shor's computation.



1. Load the x-register:
All zeros. In step 1, the computation is split up into 2^{1000} pathways, so that the wave function of the system becomes a linear superposition of all possible states, with equal phases, of the input register x.

2. Calculate f(x) requiring a single evaluation of a classical Boolean function: $\mathbf{f(x)} = c^x \pmod N$.
where N is the number to be factored, x is the value of the input register, c is any integer with no prime factors of N. The value of this function is placed in the output register y.

3. Find the period of f(x)
Shor noted that a quantum computer is very well adapted to finding the periodicity of f(x), by means of the execution of a Fourier transform on the input register x.

The Fourier transform takes a wave function of the form, $\Psi_i \rightarrow$

$$\Psi_i = \sum_{x=00\ldots0}^{11\ldots1} c_x |x\rangle$$

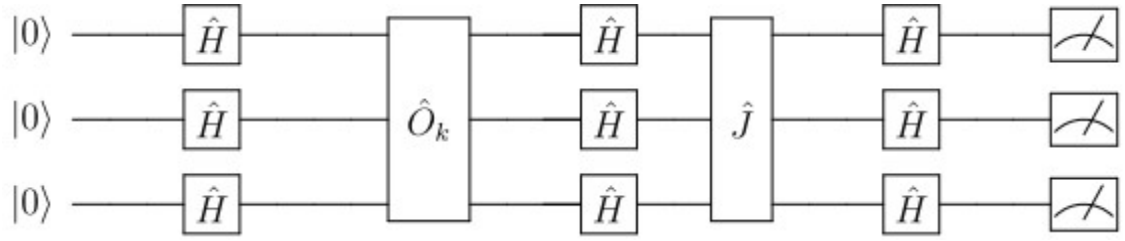
and evolves it in time so that it ends up as Ψ_f or in words, the final wave function coefficients are the discrete Fourier transform of their initial values. Shor observed that this ransformation is a unitary operation and showed that it could be performed in a number of steps polynomial in k, the number of bits in the input register (which is in turn of order the number of bits needed to represent N, the number to be factored).

$$\Psi_f = \sum_{x=00\ldots0}^{11\ldots1} \left(2^{-k/2} \sum_{x'=00\ldots0}^{11\ldots1} e^{2\pi i x x'/2^k} c_{x'} \right) |x\rangle$$

$$QFT_{mm,n} := \frac{1}{\sqrt{Q}} \cdot exp\left(i \cdot \frac{2 \cdot \pi \cdot mm \cdot n}{Q}\right)$$

XXII. Simulation of Grover's Quantum Search Algorithm

An experimental implementation of the same algorithm in Nature Communications **8**, 1918 (2017). The Grover search is implemented for N = 3 using the three qubit quantum circuit shown below. The search algorithm runs an integer number of times closest to $\frac{\pi}{4}\cdot\sqrt{2^N}$. The closest integer for N = 3 is 2. The Demonstration Calculation at the end of this Section provides a demonstration of the implementation of the J operator shown at the far right below.



There are 8 items in the data base and the oracle, **O**, identifies the correct query with a minus sign. In other words, a search of the data base should return the result |110>. The Julia and Hadamard matrices required are shown below.

$$H := \frac{1}{\sqrt{2}}\cdot\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix} \qquad O := \begin{pmatrix}1&0&0&0&0&0&0&0\\0&1&0&0&0&0&0&0\\0&0&1&0&0&0&0&0\\0&0&0&1&0&0&0&0\\0&0&0&0&1&0&0&0\\0&0&0&0&0&1&0&0\\0&0&0&0&0&0&-1&0\\0&0&0&0&0&0&0&1\end{pmatrix}$$

$$J := \begin{pmatrix}-1&0&0&0&0&0&0&0\\0&1&0&0&0&0&0&0\\0&0&1&0&0&0&0&0\\0&0&0&1&0&0&0&0\\0&0&0&0&1&0&0&0\\0&0&0&0&0&1&0&0\\0&0&0&0&0&0&1&0\\0&0&0&0&0&0&0&1\end{pmatrix}$$

Note: This is J dot

The Julia gate J is a diagonal matrix where the first diagonal element is equal to −1 and the rest are equal to 1.

$$HHH := kronecker(H, kronecker(H, H)) \qquad GroverSearch := HHH\cdot J\cdot HHH\cdot O$$

Initial Hadamard gates on the circuit wires feed the Grover search algorithm a superposition of all possible queries yielding a superposition of answers, but with the correct answer highly weighted as shown below.

$$\Psi := \frac{1}{\sqrt{8}}\cdot\begin{pmatrix}1\\1\\1\\1\\1\\1\\1\\1\end{pmatrix} \qquad GroverSearch^2\cdot\Psi = \begin{pmatrix}0.354\\0.354\\0.354\\0.354\\0.354\\0.354\\0.354\\0.354\end{pmatrix} J^2$$

This state is close to the correct result:

$$\begin{pmatrix}0\\1\end{pmatrix}\cdot\begin{pmatrix}0\\1\end{pmatrix}\cdot\begin{pmatrix}1\\0\end{pmatrix}$$

The probability of a successful search after two cycles of the circuit is $0.972^2 = 94.5\cdot\%$. For a classical search it would require on average 4 (8/2) queries. It is easy to extend the algorithm to N = 4 by adding a row to the circuit above. In this example the search of the data base should return the result |1010>.

$$O := \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

$$J' := \begin{pmatrix} -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

$$\Psi := \frac{1}{4} \cdot \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} \qquad GroverSearch^3 \cdot \Psi = \begin{pmatrix} 0.051 \\ 0.051 \\ 0.051 \\ 0.051 \\ 0.051 \\ 0.051 \\ 0.051 \\ 0.051 \\ 0.051 \\ 0.051 \\ 0.051 \\ -0.98 \\ 0.051 \\ 0.051 \\ 0.051 \\ 0.051 \\ 0.051 \end{pmatrix}$$

$$HHHH := kronecker(H, kronecker(H, kronecker(H, H)))$$

$$GroverSearch := HHHH \cdot J' \cdot HHHH \cdot O \qquad \frac{\pi}{4} \cdot \sqrt{2^4} = 3.142$$

This state is close to the correct result:

$$\begin{pmatrix} 0 \\ 1 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} \cdot \begin{pmatrix} 0 \\ 1 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

The probability of a successful search after two cycles of the circuit is $(-0.98)^2 = 96 \cdot \%$. For a classical search it would require on average 8 (16/2) queries.

Demonstration Calculation

The following calculation demonstrates the identity on the right side of Grover search circuit.
X is the NOT operator and CCZ is the controlled-controlled Z gate.

$$X := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad XXX := kronecker(X, kronecker(X, X)) \qquad CCZ := \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \end{pmatrix}$$

$$XXX \cdot CCZ \cdot XXX = \begin{pmatrix} -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \qquad J = \begin{pmatrix} -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

XXIII. An Entanglement Swapping Protocol

Physical_and_Theoretical_Chemistry, Dr. Frank Rioux

In the field of quantum information interference, superpositions and entangled states are essential resources. Entanglement, a non-factorable superposition, is routinely achieved when two photons are emitted from the same source, say a parametric down converter (PDC). Entanglement swapping involves the transfer of entanglement to two photons that were produced independently and never previously interacted. The Bell states are the four maximally entangled two-qubit entangled basis for a four-dimensional Hilbert space and play an essential role in quantum information theory and technology, including teleportation and entanglement swapping. The Bell states are shown below.

$$\Phi_p = \frac{1}{\sqrt{2}}\cdot\left[\begin{pmatrix}1\\0\end{pmatrix}\cdot\begin{pmatrix}1\\0\end{pmatrix}+\begin{pmatrix}0\\1\end{pmatrix}\cdot\begin{pmatrix}0\\1\end{pmatrix}\right] \qquad \Phi_p := \frac{1}{\sqrt{2}}\cdot\begin{pmatrix}1\\0\\0\\1\end{pmatrix} \qquad \Phi_m = \frac{1}{\sqrt{2}}\cdot\left[\begin{pmatrix}1\\0\end{pmatrix}\cdot\begin{pmatrix}1\\0\end{pmatrix}-\begin{pmatrix}0\\1\end{pmatrix}\cdot\begin{pmatrix}0\\1\end{pmatrix}\right] \qquad \Phi_m := \frac{1}{\sqrt{2}}\cdot\begin{pmatrix}1\\0\\0\\-1\end{pmatrix}$$

$$\Psi_p = \frac{1}{\sqrt{2}}\cdot\left[\begin{pmatrix}1\\0\end{pmatrix}\cdot\begin{pmatrix}0\\1\end{pmatrix}+\begin{pmatrix}1\\0\end{pmatrix}\cdot\begin{pmatrix}0\\1\end{pmatrix}\right] \qquad \Psi_p := \frac{1}{\sqrt{2}}\cdot\begin{pmatrix}0\\1\\1\\0\end{pmatrix} \qquad \Psi_m = \frac{1}{\sqrt{2}}\cdot\left[\begin{pmatrix}1\\0\end{pmatrix}\cdot\begin{pmatrix}0\\1\end{pmatrix}-\begin{pmatrix}0\\1\end{pmatrix}\cdot\begin{pmatrix}1\\0\end{pmatrix}\right] \qquad \Psi_m := \frac{1}{\sqrt{2}}\cdot\begin{pmatrix}0\\1\\-1\\0\end{pmatrix}$$

A four-qubit state is prepared in which photons 1 and 2 are entangled in Bell state Φ_p, and photons 3 and 4 are entangled in Bell state Ψ_m. The state multiplication below is understood to be tensor vector multiplication.

$$\Psi = \Phi_p\cdot\Psi_m = \frac{1}{\sqrt{2}}\cdot\begin{pmatrix}1\\0\\0\\1\end{pmatrix}\cdot\frac{1}{\sqrt{2}}\cdot\begin{pmatrix}0\\1\\-1\\0\end{pmatrix} \qquad \Psi := \frac{1}{2}\cdot(0\ \ 1\ \ -1\ \ 0\ \ 0\ \ 0\ \ 0\ \ 0\ \ 0\ \ 0\ \ 0\ \ 0\ \ 0\ \ 1\ \ -1\ \ 0)^T$$

$$I := \begin{pmatrix}1&0\\0&1\end{pmatrix}$$

Four Bell state measurements are now made on photons 2 and 3 which entangles photons 1 and 4.
Projection of photons 2 and 3 onto Φ_p projects photons 1 and 4 onto Ψ_m.

$$\left(kronecker\left(I, kronecker\left(\Phi_p\cdot\Phi_p{}^T, I\right)\right)\cdot\Psi\right)^T = (0\ \ 0.25\ \ 0\ \ 0\ \ 0\ \ 0\ \ 0\ \ 0.25\ \ -0.25\ \ 0\ \ 0\ \ 0\ \ 0\ \ 0\ \ -0.25\ \ 0)$$

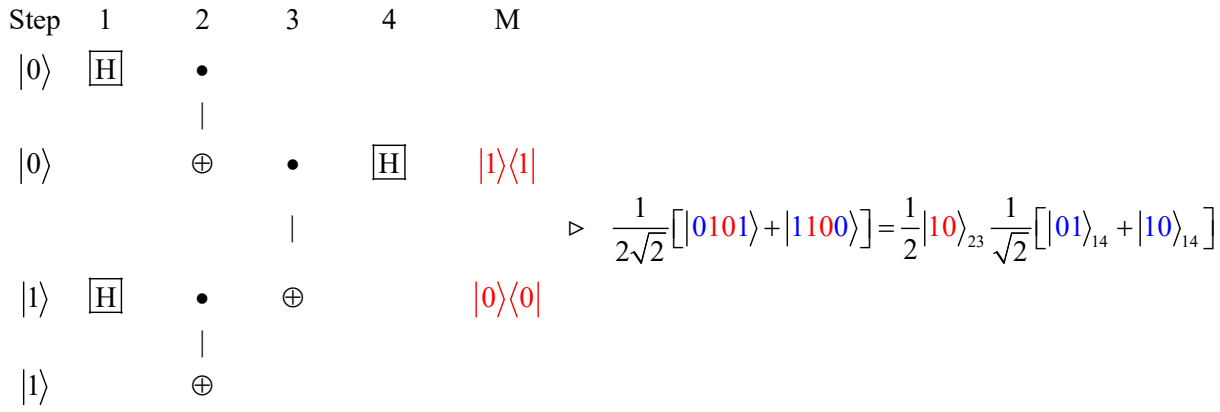
$$\frac{1}{2\cdot\sqrt{2}}\cdot\left[\begin{pmatrix}1\\0\end{pmatrix}\cdot\frac{1}{\sqrt{2}}\cdot\begin{pmatrix}1\\0\\0\\1\end{pmatrix}\cdot\begin{pmatrix}0\\1\end{pmatrix}-\begin{pmatrix}0\\1\end{pmatrix}\cdot\frac{1}{\sqrt{2}}\cdot\begin{pmatrix}1\\0\\0\\1\end{pmatrix}\cdot\begin{pmatrix}1\\0\end{pmatrix}\right]^T = \frac{1}{4}\cdot(0\ \ 1\ \ 0\ \ 0\ \ 0\ \ 0\ \ 0\ \ 1\ \ -1\ \ 0\ \ 0\ \ 0\ \ 0\ \ 0\ \ -1\ \ 0)$$

Projection of photons 2 and 3 onto Φ_m projects photons 1 and 4 onto Ψ_p.

$$\left(kronecker\left(I, kronecker\left(\Phi_m \cdot \Phi_m^{\,T}, I\right)\right) \cdot \Psi\right)^T = (0 \;\; 0.25 \;\; 0 \;\; 0 \;\; 0 \;\; 0 \;\; 0 \;\; -0.25 \;\; 0.25 \;\; 0 \;\; 0 \;\; 0 \;\; 0 \;\; 0 \;\; -0.25 \;\; 0)$$

$$\frac{1}{2\cdot\sqrt{2}} \cdot \left[\begin{pmatrix} 1 \\ 0 \end{pmatrix} \cdot \frac{1}{\sqrt{2}} \cdot \begin{pmatrix} 1 \\ 0 \\ 0 \\ -1 \end{pmatrix} \cdot \begin{pmatrix} 0 \\ 1 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \end{pmatrix} \cdot \frac{1}{\sqrt{2}} \cdot \begin{pmatrix} 1 \\ 0 \\ 0 \\ -1 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} \right]^T = \frac{1}{4} \cdot (0 \;\; 1 \;\; 0 \;\; 0 \;\; 0 \;\; 0 \;\; 0 \;\; -1 \;\; 1 \;\; 0 \;\; 0 \;\; 0 \;\; 0 \;\; 0 \;\; -1 \;\; 0)$$

Here's a quantum circuit that accomplishes this entanglement swap.



Projection of photons 2 and 3 onto Ψ_p projects photons 1 and 4 onto -Φ_m.

$$\left(kronecker\left(I, kronecker\left(\Psi_p \cdot \Psi_p^{\,T}, I\right)\right) \cdot \Psi\right)^T = (0 \;\; 0 \;\; -0.25 \;\; 0 \;\; -0.25 \;\; 0 \;\; 0 \;\; 0 \;\; 0 \;\; 0 \;\; 0 \;\; 0.25 \;\; 0 \;\; 0.25 \;\; 0 \;\; 0)$$

$$\frac{1}{2\cdot\sqrt{2}} \cdot \left[\begin{pmatrix} 0 \\ 1 \end{pmatrix} \cdot \frac{1}{\sqrt{2}} \cdot \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix} \cdot \begin{pmatrix} 0 \\ 1 \end{pmatrix} - \begin{pmatrix} 1 \\ 0 \end{pmatrix} \cdot \frac{1}{\sqrt{2}} \cdot \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} \right]^T = \frac{1}{4} \cdot (0 \;\; 0 \;\; -1 \;\; 0 \;\; -1 \;\; 0 \;\; 0 \;\; 0 \;\; 0 \;\; 0 \;\; 0 \;\; 1 \;\; 0 \;\; 1 \;\; 0 \;\; 0)$$

Finally, projection of photons 2 and 3 onto Ψ_m projects photons 1 and 4 onto Φ_p.

$$\left(kronecker\left(I, kronecker\left(\Psi_m \cdot \Psi_m^{\,T}, I\right)\right) \cdot \Psi\right)^T = (0 \;\; 0 \;\; -0.25 \;\; 0 \;\; 0.25 \;\; 0 \;\; 0 \;\; 0 \;\; 0 \;\; 0 \;\; 0 \;\; -0.25 \;\; 0 \;\; 0.25 \;\; 0 \;\; 0)$$

$$\frac{-1}{2\cdot\sqrt{2}} \cdot \left[\begin{pmatrix} 1 \\ 0 \end{pmatrix} \cdot \frac{1}{\sqrt{2}} \cdot \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \end{pmatrix} \cdot \frac{1}{\sqrt{2}} \cdot \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix} \cdot \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right]^T = \frac{1}{4} \cdot (0 \;\; 0 \;\; -1 \;\; 0 \;\; 1 \;\; 0 \;\; 0 \;\; 0 \;\; 0 \;\; 0 \;\; 0 \;\; -1 \;\; 0 \;\; 1 \;\; 0 \;\; 0)$$

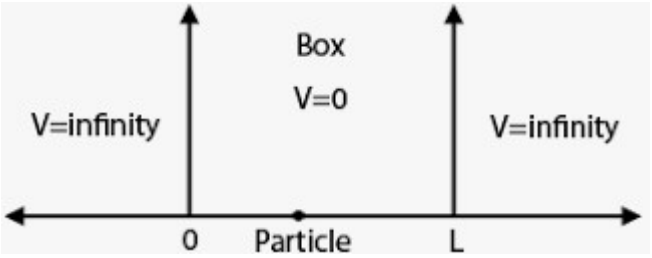
XXIV. Quantum Mechanical Calculations Illuminated with Dirac Notation

The following example is from "*PHYSICAL CHEMISTRY for the Chemical Sciences*", Raymond Chang"

A Particle in a Box in a One Dimensional Box

At the end of the nineteenth century, there were new experimental results that could not be explained by the so-called classical theories of physics. In 1900, the German physicist Max Planck proposed the quantum theory to explain one of these experiments. In this chapter, we take a historical approach and follow the early development of quantum theory.

Consider a particle of mass m confined to a one-dimensional box of length L. We again assume that the particle has zero potential energy inside the box ^ or on the line segment h ; that is, V = 0. The particle has only kinetic energy. At each end of the box is a wall of infinite potential energy, so there is no probability of finding the particle at the walls or outside the box. For simplicity, we chose the line segment to start at the origin, so x is restricted by $0 \le x \le L$, See Figure below. The Schrödinger equation is similar to that for the free particle, with the difference being that the value of x is constrained by the size of the box.



$$\frac{-\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x) \qquad 0 \le x \le L$$

For the particle-in-a-box Schrödinger equation, let us try a trial wave function,

$$\psi(x) = A\sin(kx) + B\cos(kx)$$

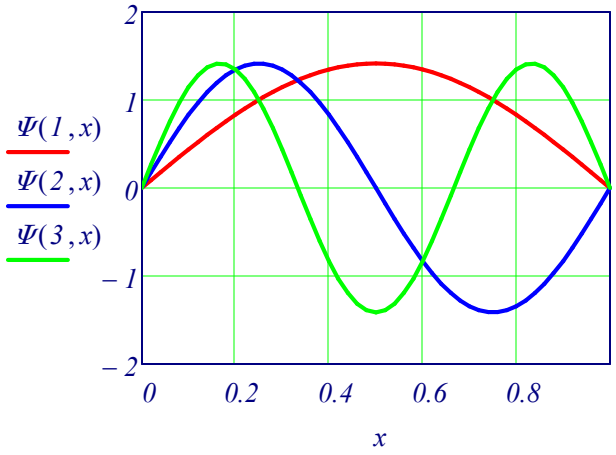
The particle-in-a-box (PIB) problem is exactly soluble and the solution is calculated below for the first 20 eigenstates. All calculations will be carried out in atomic units (h = 2π) for a particle of unit mass in a 1 D box.

$n := 1 .. 20$ $\qquad \Psi(n,x) := \sqrt{2}\cdot\sin(n\cdot\pi\cdot x)$ $\qquad E_n := \frac{n^2\cdot\pi^2}{2}$

The first five energy eigenvalues are:

$E_1 = 4.935$ $\qquad E_2 = 19.739$ $\qquad E_3 = 44.413$ $\qquad E_4 = 78.957$ $\qquad E_5 = 123.37$

The first three eigenfunctions are displayed below. $x := 0, .02 .. 1$



The PIB eigenfunctions form a complete basis set, and therefore other functions can be written as linear combinations in this basis set. For example, Φ, χ, and Γ are three trial functions that satisfy the boundary conditions for the particle in a 1 bohr box.

$$\Phi(x) := \sqrt{30}\cdot\left(x - x^2\right) \qquad \chi(x) := \sqrt{105}\cdot\left(x^2 - x^3\right) \qquad \Gamma(x) := \sqrt{105}\cdot x\cdot(1-x)^2$$

In Dirac bracket notation we can express each of these functions as a linear combination in the basis set. For example, for Φ we have,

$$\langle x|\Phi\rangle = \sum_n \langle x|\Psi_n\rangle\langle\Psi_n|\Phi\rangle = \sum_n \langle x|\Psi_n\rangle\int_0^1 \langle\Psi_n|x\rangle\langle x|\Phi\rangle dx = \sum_n \Psi_n(x)\int_0^1 \Psi_n^*(x)\Phi(x)dx = \sum_n \Psi_n(x)a_n$$

Here both the finite and continuous completeness relations have been used:

$$\sum_n |\Psi_n\rangle\langle\Psi_n| = 1 \quad \text{and} \quad \int |x\rangle\langle x|\,dx = 1$$

The various overlap integrals for the three trial function (a_n, b_n, and c_n) are evaluated below.

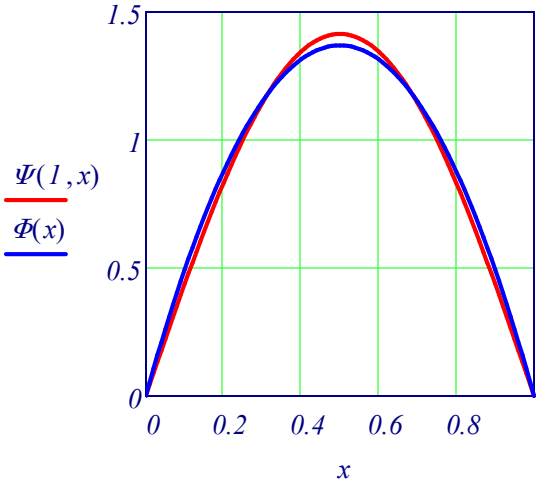
$$a_n := \int_0^1 \Psi(n,x)\cdot\Phi(x)\,dx \qquad b_n := \int_0^1 \Psi(n,x)\cdot\chi(x)\,dx \qquad c_n := \int_0^1 \Psi(n,x)\cdot\Gamma(x)\,dx$$

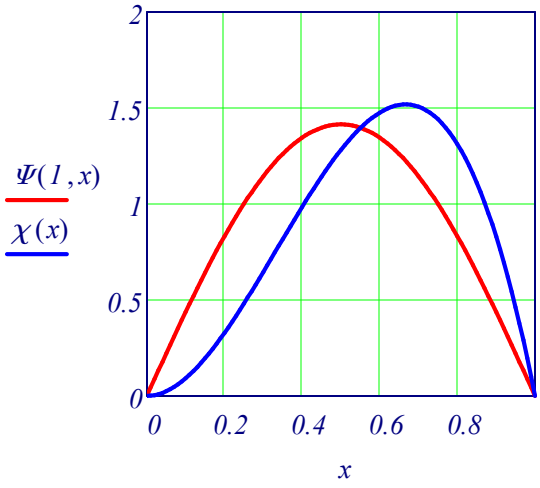
As shown above, these overlap integrals are set up as follows:

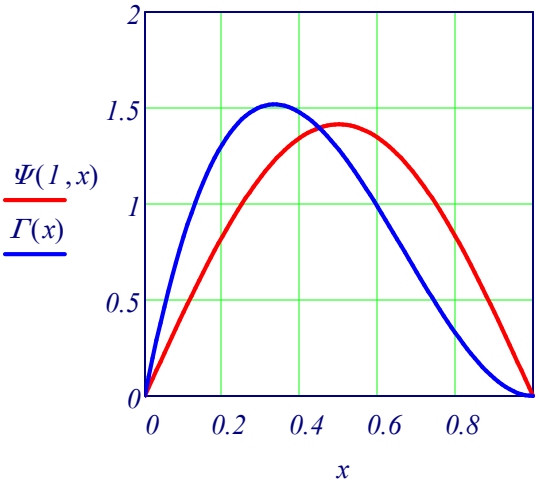
$$a_n = \langle\Psi_n|\Phi\rangle = \int_0^1 \langle\Psi_n|x\rangle\langle x|\Phi\rangle dx = \int_0^1 \Psi_n^*(x)\Phi(x)dx$$

The figures shown below demonstrate that only Φ is a reasonable representative for the ground state wavefunction.

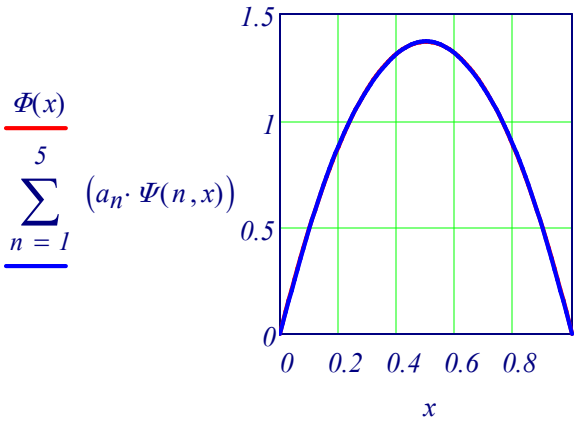
$x := 0, .01 .. 1$



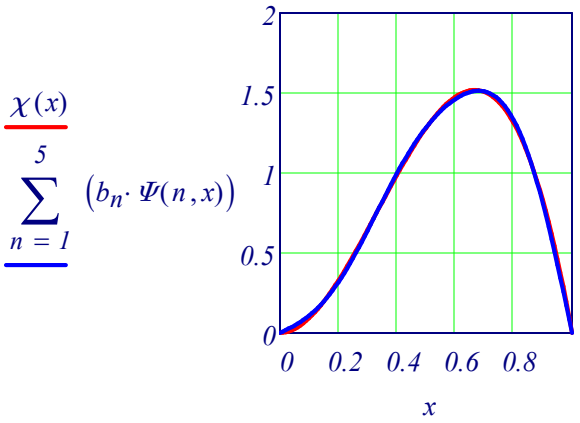


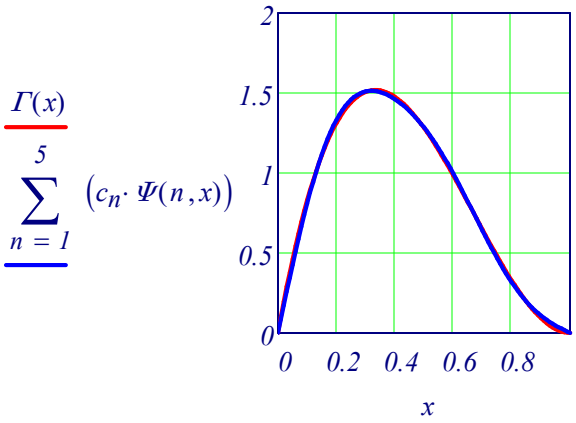


However, if Φ is written as a linear combination of the first 5 PIB eigenfunctions, one gets two functions that are essentially indistinguishable from one another.



The same, of course, is true for χ and Γ, as is demonstrated in the graphs shown below.





Traditionally we use energy as a criterion for the quality of a trial wavefunction by evaluating the variational integral in the following way. Φ(x) is the best trial function because it gives the lowest energy.

$$\int_0^1 \Phi(x)\cdot -\frac{1}{2}\cdot\frac{d^2}{dx^2}\Phi(x)\,dx = 5 \qquad \int_0^1 \chi(x)\cdot -\frac{1}{2}\cdot\frac{d^2}{dx^2}\chi(x)\,dx = 7 \qquad \int_0^1 \Gamma(x)\cdot -\frac{1}{2}\cdot\frac{d^2}{dx^2}\Gamma(x)\,dx = 7$$

With Dirac notation we would write:

$$\langle E\rangle = \langle\Phi|\hat{H}|\Phi\rangle = \sum_n \langle\Phi|\hat{H}|\Psi_n\rangle\langle\Psi_n|\Phi\rangle = \sum_n \langle\Phi|\Psi_n\rangle E_n \langle\Psi_n|\Phi\rangle = \sum_n a_n^2 E_n$$

Thus we easily show the same result.

$$\sum_n \left[(a_n)^2\cdot E_n\right] = 5 \qquad \sum_n \left[(b_n)^2\cdot E_n\right] = 6.999 \qquad \sum_n \left[(c_n)^2\cdot E_n\right] = 6.999$$

We now show, belatedly, that the three trial functions are normalized by both methods.

$$\int_0^1 \Phi(x)^2\,dx = 1 \qquad \int_0^1 \chi(x)^2\,dx = 1 \qquad \int_0^1 \Gamma(x)^2\,dx = 1$$

In Dirac bracket notation this is written as: $\langle\Phi|\Phi\rangle = \sum_n \langle\Phi|\Psi_n\rangle\langle\Psi_n|\Phi\rangle = \sum_n a_n^2$

$$\sum_n (a_n)^2 = 1 \qquad \sum_n (b_n)^2 = 1 \qquad \sum_n (c_n)^2 = 1$$

We now calculate some over-lap integrals:

$$\int_0^1 \Phi(x)\cdot\chi(x)\,dx = 0.935 \qquad \int_0^1 \Phi(x)\cdot\Gamma(x)\,dx = 0.935 \qquad \int_0^1 \chi(x)\cdot\Gamma(x)\,dx = 0.75$$

In Dirac notation this is formulated as: $\langle\Phi|\Gamma\rangle = \sum_n \langle\Phi|\Psi_n\rangle\langle\Psi_n|\Gamma\rangle = \sum_n a_n c_n$

$$\sum_n (a_n\cdot b_n) = 0.935 \qquad \sum_n (a_n\cdot c_n) = 0.935 \qquad \sum_n (b_n\cdot c_n) = 0.75$$

As a final exercise we calculate the expectation value for position using the three trial wave functions. In bracket notation this calculation is set up most directly as follows.

$$\langle\Phi|\hat{x}|\Phi\rangle = \int_0^1 \langle\Phi|\hat{x}|x\rangle\langle x|\Phi\rangle\,dx = \int_0^1 \langle\Phi|x\rangle x\langle x|\Phi\rangle\,dx = \int_0^1 \Phi(x)^* x\,\Phi(x)dx$$

where we have employed the eigenvalue equation for the position operator: $\hat{x}|x\rangle = |x\rangle x$

Evaluation of the integral on the right for each trial function is shown below. Naturally the results are consistent with the shapes of the trial wave functions shown in the first figure.

$$\int_0^1 \Phi(x)\cdot x\cdot \Phi(x)\,dx = 0.5 \qquad \int_0^1 \chi(x)\cdot x\cdot \chi(x)\,dx = 0.625 \qquad \int_0^1 \Gamma(x)\cdot x\cdot \Gamma(x)\,dx = 0.375$$

Although it is computationally less expedient, it is instructive to expand these calculations in terms of the PIB eigenfunctions.

$$\langle \Phi | \hat{x} | \Phi \rangle = \sum_m \sum_n \int_0^1 \langle \Phi | \Psi_m \rangle \langle \Psi_m | x \rangle x \langle x | \Psi_n \rangle \langle \Psi_n | \Phi \rangle dx = \sum_m \sum_n a_m^* a_n \int_0^1 \sqrt{2}\sin(m\pi x) x \sqrt{2}\sin(n\pi x)\,dx$$

Truncating the calculation after five PIB eigenfunctions yields the same results as obtained with the integrals above.

$$\sum_{m=1}^{5}\sum_{n=1}^{5}\left(a_m\cdot a_n\cdot\int_0^1 \sqrt{2}\cdot\sin(m\cdot\pi\cdot x)\cdot x\cdot\sqrt{2}\cdot\sin(n\cdot\pi\cdot x)\,dx\right) = 0.5$$

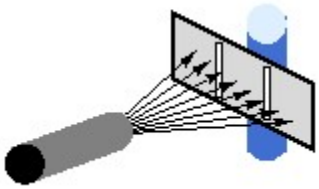
$$\sum_{m=1}^{5}\sum_{n=1}^{5}\left(b_m\cdot b_n\cdot\int_0^1 \sqrt{2}\cdot\sin(m\cdot\pi\cdot x)\cdot x\cdot\sqrt{2}\cdot\sin(n\cdot\pi\cdot x)\,dx\right) = 0.625$$

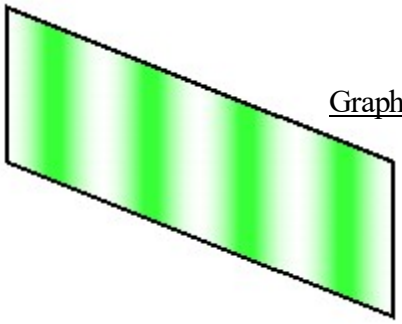
$$\sum_{m=1}^{5}\sum_{n=1}^{5}\left(c_m\cdot c_n\cdot\int_0^1 \sqrt{2}\cdot\sin(m\cdot\pi\cdot x)\cdot x\cdot\sqrt{2}\cdot\sin(n\cdot\pi\cdot x)\,dx\right) = 0.375$$

XXV. Simulating the Aharonov–Bohm Effect - Wikipedia

The Aharonov–Bohm effect is a quantum-mechanical phenomenon in which an electrically charged particle is influenced by the vector potential **A** in regions in which the magnetic field **B** is zero. A beam of monoenergetic electrons passes through a double slit on opposite sides of a solenoid. In QM, the same particle can travel between two paths. The expected interference pattern of the waves going through the two slits is shifted by an additional phase difference **ϕ** when the solenoid encloses a magnetic field, despite the magnetic field being zero in the regions through which the electrons pass. This can be observed experimentally by the horizontal displacement of the interference fringes.

Aharonov–Bohm Effect Apparatus





Graphic from Wikipedia

Note: The same pattern occurs when light goes through a double slit.

Illustration of how double-slit experiment in which Aharonov–Bohm effect can be observed: electrons pass through two slits, interfering at an observation screen, with the interference pattern shifted when a magnetic field B is turned on in the cylindrical solenoid. **The effect on the interference fringes is calculated and displayed below.**

Slit Positions $x_L := 1 \quad x_R := 2$

Slit Width $\delta := 0.2$

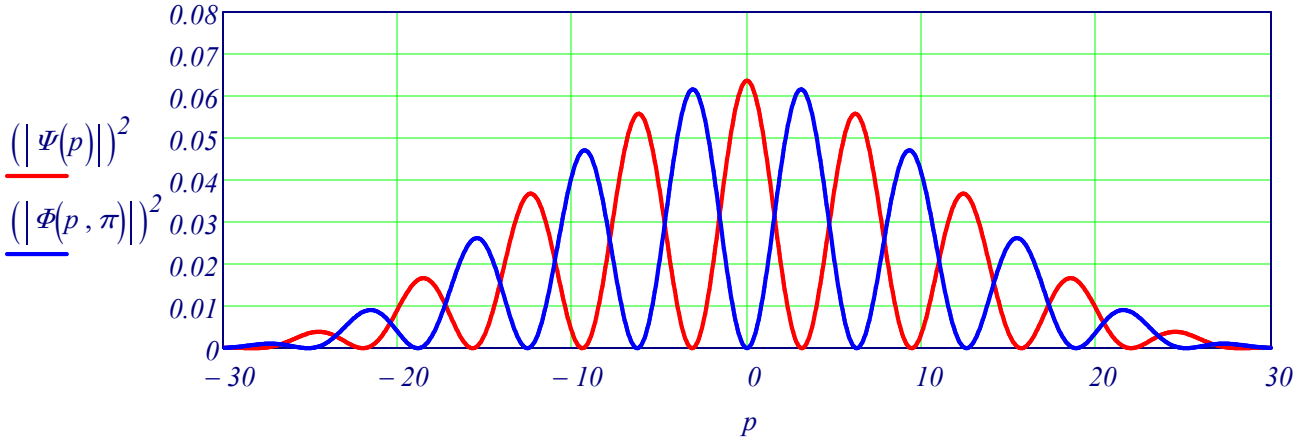
AB Relative Phase Shift

Phase $\phi := \pi$ for $exp(i\cdot\phi)$

$$\Psi(p) := \frac{1}{\sqrt{2}}\left(\int_{x_L-\frac{\delta}{2}}^{x_L+\frac{\delta}{2}} \frac{1}{\sqrt{2\cdot\pi}}\cdot exp(-i\cdot p\cdot x)\cdot\frac{1}{\sqrt{\delta}}\,dx + \int_{x_R-\frac{\delta}{2}}^{x_R+\frac{\delta}{2}} \frac{1}{\sqrt{2\cdot\pi}}\cdot exp(-i\cdot p\cdot x)\cdot\frac{1}{\sqrt{\delta}}\,dx\right)$$

$$\Phi(p,\phi) := \frac{1}{\sqrt{2}}\left(\int_{x_L-\frac{\delta}{2}}^{x_L+\frac{\delta}{2}} \frac{1}{\sqrt{2\cdot\pi}}\cdot exp(-i\cdot p\cdot x)\cdot\frac{1}{\sqrt{\delta}}\,dx + exp(i\cdot\phi)\cdot\int_{x_R-\frac{\delta}{2}}^{x_R+\frac{\delta}{2}} \frac{1}{\sqrt{2\cdot\pi}}\cdot exp(-i\cdot p\cdot x)\cdot\frac{1}{\sqrt{\delta}}\,dx\right)$$

Aharonov–Bohm Effect Interference Pattern with 180 degree Phase Difference



XXVI. QM: Schrödinger Wavefunction, Matrix, and Wigner Phase Space

We will model three Formulations of Quantum Mechanics:

Schrödinger Wavefunction, Matrix, and Wigner Phase Space

There are seven commonly used nonrelativistic formulations for quantum mechanics. These are the wavefunction, matrix, path integral, phase space, density matrix, second quantization, variational, formulations. Also mentioned are the many-worlds and transactional interpretations. The various formulations differ dramatically in mathematical and conceptual overview, yet each one makes identical predictions for all experimental results.

A. The matrix formulation (Heisenberg)

The matrix formulation of quantum mechanics, developed by Werner Heisenberg in June of 1925, was the first formulation to be uncovered. The wavefunction formulation, which enjoys wider currency today, was developed by Erwin Schrödinger about six months later.

B. The wavefunction formulation (Schrödinger)

Compared to the matrix formulation, the wavefunction formulation of quantum mechanics shifts the focus from "measurable quantity" to "state." The state of a system with two particles ~ ignoring spin ! is represented mathematically by a complex function in six-dimensional configuration space, namel .

C. Phase space formulation - See Section XXIV: The Wigner Quasiprobability Distribution)

For a single particle restricted to one dimension, the Wigner phase-space distribution function is

$$W(x,p,t)=\frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty}\psi^*(x-\tfrac{1}{2}y,t)\times\psi(x+\tfrac{1}{2}y,t)e^{-ipy/\hbar}\,dy$$

D. The path integral formulation (Feynman)

The path integral formulation (also called the sum-over-histories formulation) shifts the focus from "state" to "transition probability."

E. Density matrix formulation

The density matrix corresponding to a pure state $|\psi\rangle$ is the outer product $\hat{\rho}=|\psi\rangle\langle\psi|$

Given the density matrix p^, the quantal state $|\psi\rangle$ can be found as follows: First select an arbitrary state $|\phi\rangle$. The unnormalized ket $|\psi\rangle$ is p^$|\phi\rangle$ (as long as this quantity does not vanish).

F. Second quantization formulation This formulation features operators that create and destroy particles. It was developed in connection with quantum fixed theory, where such actions are physical effects ~ for example, an electron and a positron are destroyed and a photon is created ! .

G. Variational formulation

The "variational formulation" must not be confused with the more-commonly-encountered "variational method", which provides a bound on the ground state energy. Instead the variational formulation provides a full picture describing any state—not just the ground state—and dictating its full time evolution—not just its energy. It is akin to Hamilton's principle in classical mechanics.

XXVII. Solution of Schrödinger Wave Equation for Propagation of an Electron

Given an electron of mass, m_e, velocity, v_e, kinetic energy of 1 eV

By Quantum Mechanics. it has an associated de Broglie wavelength, λ_e, and wavenumber k_0

Planck's Constant: $h := 6.626 \cdot 10^{-34} J \cdot s$

Given: $m_e := 9.10938 \cdot 10^{-31} kg$ $v := 1 \cdot 10^{3} \frac{m}{s}$ $T := 1 eV$ $\lambda_e := \frac{h}{\sqrt{2 \cdot m_e \cdot T}} = 12.265 \cdot A$

Consider a monochromatic E Field plane wave associated with an electron which propagates in an isotropic and homogeneous medium: $E(r,t) = E_0 \cdot e^{[i \cdot (k \cdot r - \omega \cdot t)]}$

Associated with this electron is a wavenumber, k_e, amplitude, A

$k_e := 8.637 \cdot 10^{6} \cdot \frac{1}{m}$ $A := \frac{1}{\sqrt{a \cdot \sqrt{\pi}}}$ $h_{bar} := \frac{h}{2 \cdot \pi}$ $A_m := A \cdot \sqrt{m}$

$eV := 1.602 \cdot 10^{-19} J$

The electron has Kinetic Energy: $E := \frac{h_{bar}^{2} \cdot k_e^{2}}{2 m_e}$ $E = 4.554 \times 10^{-25} J$ **Electron Frequency:** $\omega = 2 \pi \cdot f$

Equation of Traveling Wave: $\psi(x) = A \cdot e^{i \cdot (k \cdot x - \omega \cdot t)} + B \cdot e^{-i \cdot (k \cdot x + \omega \cdot t)}$

To solve the one-dimensional Schrödinger equation for a free particle of mass m moving with velocity v, we can proceed a follows:

Solve Schrödinger's Wave Equation for the Quantum Wavefunction, Ψ(x, t)

$$\frac{-\hbar^2}{2 \cdot m_e} \cdot \frac{\partial^2}{\partial x^2} \Psi = i \cdot \hbar \cdot \frac{\partial}{\partial t} \Psi$$

$$\Psi(x,t) = \int_{-\infty}^{\infty} \psi(k,x,t)\, dk$$

$$\Psi(x,t) = \frac{A \cdot a}{\sqrt{2\pi}} \cdot \int_{-\infty}^{\infty} exp\left[\frac{-1}{2} a^2 \cdot (k - k_0)^2 + i \cdot k \cdot x - \frac{i \cdot h_{bar} \cdot t}{2 \cdot m_e} \cdot k^2 \right] dk$$

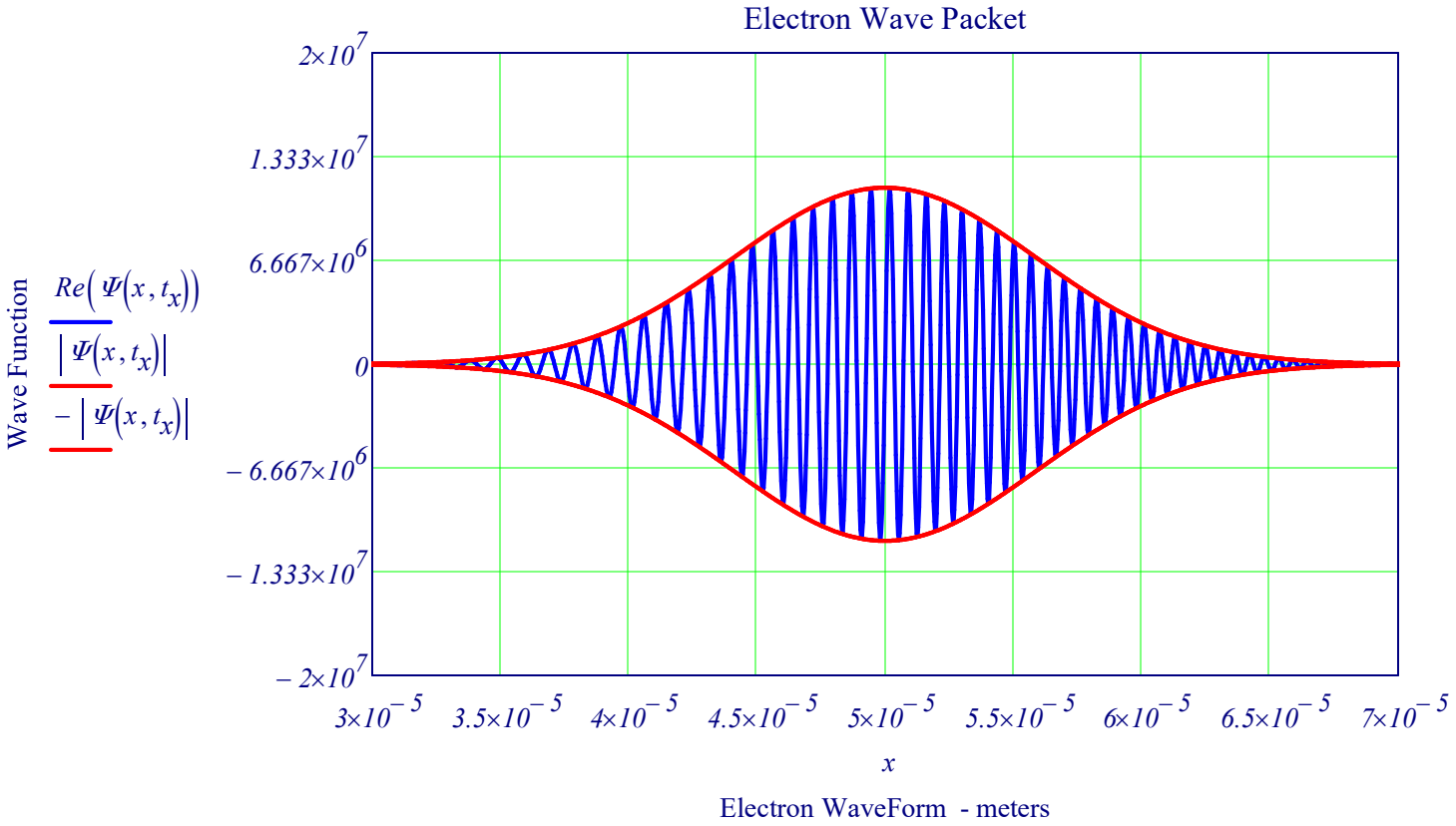
Evaluate the Wavefunction over the Space and Time Region: $a := 1 \cdot \mu m$ $t_x := 50 ns$

Solution for Ψ(x,t):

$$\Psi(x,t) := \frac{A_m}{\sqrt{1 + \frac{i \cdot h_{bar} \cdot t}{m_e \cdot a^2}}} \cdot exp\left[\frac{-\left(x^2 - 2 \cdot i \cdot a^2 \cdot k_e \cdot x + \frac{i \cdot h_{bar} \cdot t}{2 m_e} \cdot k_e^{2} \cdot a^2 \right)}{2 \cdot a^2 \cdot \left(1 + \frac{i \cdot h_{bar} \cdot t}{m_e \cdot a^2} \right)} \right]$$

Plot Wavefunction Ψ(x,t) over Distance Range, x

Distance Range: $x := 10^{-5}\cdot 2m\,,\,10^{-5}\cdot 2m + \left(\frac{10^{-5}\cdot 8\cdot m - 10^{-5}\cdot 2m}{2000}\right) .. 10^{-5}\cdot 8m$



Numerical Schrödinger Equation Solutions for 3-D Harmonic Oscillator

Parameters:

$E := 7.5$ $L := 0$

Reduced mass: $\mu := 1$ Angular momentum: $L := 0$ Integration limit: $r_{max} := 6$ $r := 0, 0.01 .. r_{max}$

Force constant: $k := 1$

Solve Schrödinger's equation numerically. Use Mathcad's ODE solve block:

Given

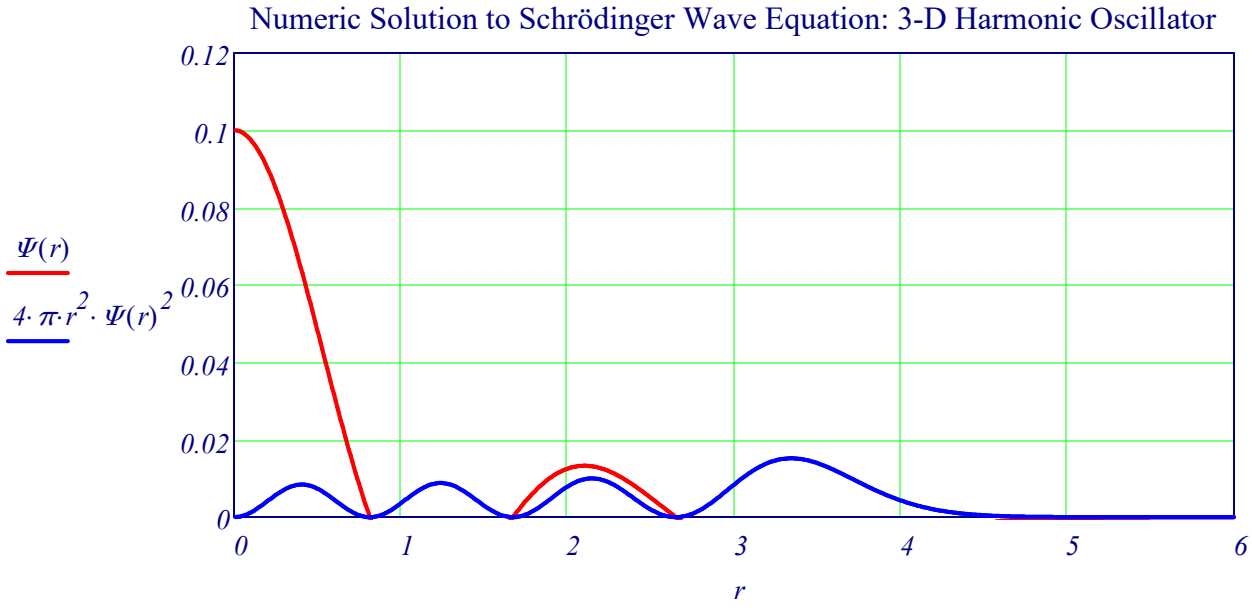
$$\frac{-1}{2\cdot\mu}\cdot\frac{d^2}{dr^2}\Psi(r) - \frac{1}{r\cdot\mu}\cdot\frac{d}{dr}\Psi(r) + \left[\frac{L\cdot(L+1)}{2\cdot\mu\cdot r^2} + \frac{1}{2}\cdot k\cdot r^2\right]\cdot\Psi(r) = E\cdot\Psi(r)$$

$$\Psi(.001) = .1 \qquad \Psi'(.001) = .1$$

$$\Psi := Odesolve(r, r_{max})$$

Energy guess: $E \equiv 7.5$

Normalize the wavefunction: $\Psi(r) := \left(\int_0^{r_{max}} \Psi(r)^2\cdot 4\cdot\pi\cdot r^2\, dr\right)^{\frac{-1}{2}}\cdot\Psi(r)$



XXVIII. Basic Quantum Mechanics in Coordinate, Momentum & Phase Space

Tutorial: *The Wigner Quasiprobability Distribution*, Wikipedia

The Wigner quasiprobability distribution (also called the Wigner function or the Wigner–Ville distribution, after Eugene Wigner and Jean-André Ville) is a quasiprobability distribution. It was introduced by Eugene Wigner in 1932 to study quantum corrections to classical statistical mechanics. The goal was to link the wavefunction that appears in Schrödinger's equation to a probability distribution in phase space.

It is a generating function for all spatial autocorrelation functions of a given quantum-mechanical wavefunction ψ(x). Thus, it maps on the quantum density matrix in the map between real phase-space functions and Hermitian operators introduced by Hermann Weyl in 1927, in a context related to representation theory in mathematics (see Weyl quantization). In effect, it is the Wigner–Weyl transform of the density matrix, so the realization of that operator in phase space.

In 1949, José Enrique Moyal, who had derived it independently, recognized it as the quantum moment-generating functional, and thus as the basis of an elegant encoding of all quantum expectation values, and hence quantum mechanics, in phase space.

Relation to classical mechanics

A classical particle has a definite position and momentum, and **hence it is represented by a point in phase space**. Given a collection (ensemble) of particles, the probability of finding a particle at a certain position in phase space is specified by a probability distribution, the Liouville density. **This strict interpretation fails for a quantum particle, due to the uncertainty principle.** Instead, the above quasiprobability Wigner distribution plays an analogous role, but does not satisfy all the properties of a conventional probability distribution; and, conversely, satisfies boundedness properties unavailable to classical distributions.

For instance, the Wigner distribution can and normally does take on negative values for states which have no classical model—and is a **convenient indicator of quantum-mechanical interference.** (See below for a characterization of pure states whose Wigner functions are non-negative.) Smoothing the Wigner distribution through a filter of size larger than ħ (e.g., convolving with a phase-space Gaussian, a Weierstrass transform, to yield the Husimi representation, below), results in a positive-semidefinite function, i.e., it may be thought to have been coarsened to a semi-classical one.

Regions of such negative value are provable (by convolving them with a small Gaussian) to be "small": they cannot extend to compact regions larger than a few ħ, and hence disappear in the classical limit. They are shielded by the uncertainty principle, which does not allow precise location within phase-space regions smaller than ħ, and thus renders such "negative probabilities" less paradoxical.

Definition and meaning

The Wigner distribution W(x,p) of a pure state is defined as

$$W(x,p) \stackrel{\text{def}}{=} \frac{1}{\pi\hbar}\int_{-\infty}^{\infty} \psi^*(x+y)\psi(x-y)e^{2ipy/\hbar}\,dy,$$

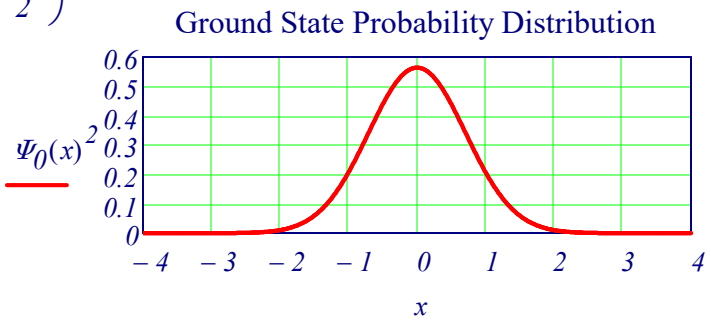
where ψ is the wavefunction, and x and p are position and momentum, but could be any conjugate variable pair (e.g. real and imaginary parts of the electric field or frequency and time of a signal). Note that it may have support in x even in regions where ψ has no support in x ("beats"). It is symmetric in x and p: See the Phase Space Distribution of the Wigner Function Expressed in Dirac Notation shown on the following page.

Ground State Probability Distribution for a Harmonic Oscillator: Math

We will use calculations on the harmonic oscillator to illustrate the relationship between the coordinate, momentum and phase space representations of quantum mechanics.
The first (ground state) oscillator eigenfunction is given below.

$$\Psi_0(x) := \pi^{\frac{-1}{4}} \cdot exp\left(\frac{-x^2}{2}\right) \qquad x := -4, -3.99 .. 4$$

As is well-known, in coordinate space the position operator is multiplicative and the momentum operator is differential. In momentum space it is the reverse, while in phase space, both position and momentum are multiplicative operators.



$$\int_{-\infty}^{\infty} \Psi_0(x)^2 dx = 1 \qquad x_{ave} = \int_{-\infty}^{\infty} x \cdot \Psi_0(x)^2 dx \to 0 \qquad x2_{ave} := \int_{-\infty}^{\infty} x^2 \cdot \Psi_0(x)^2 dx \to \frac{1}{2}$$

$$p_{ave} := \int_{-\infty}^{\infty} \Psi_0(x) \cdot \frac{1}{i} \cdot \frac{d}{dx} \Psi_0(x) dx \to 0 \qquad p2_{ave} := \int_{-\infty}^{\infty} \Psi_0(x) \cdot \frac{d^2}{dx^2} \Psi_0(x) dx \to \frac{1}{2}$$

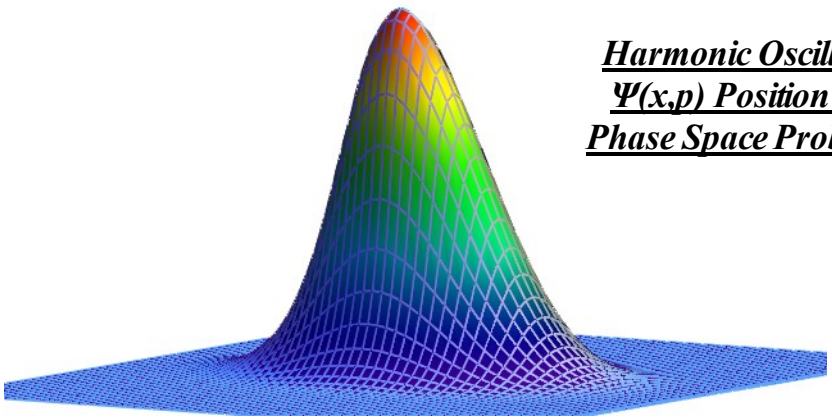
Phase Space Distribution Calculations: The Wigner Quasiprobability Distribution for a Harmonic Oscillator

Phase-space calculations require a Phase-Space Distribution, such as the Wigner function. Because this approach to quantum mechanics is not as familiar as the Schrödinger formulation, several important equations will be deconstructed using Dirac notation. **Expressed in Dirac Notation, the Wigner Function resembles a classical trajectory.**

$$W(x,p) = \int_{-\infty}^{\infty} \left\langle \Psi | x + \frac{s}{2} \right\rangle \left\langle x + \frac{s}{2} | p \right\rangle \left\langle p | x - \frac{s}{2} \right\rangle \left\langle x - \frac{s}{2} | \Psi \right\rangle ds \qquad W_0(x,p) := \frac{1}{\pi} \cdot e^{\left(-x^2\right) - p^2}$$

The four Dirac brackets are read from right to left as follows: (1) is the amplitude that a particle state Ψ has at position (x - s/2); 2 is the amplitude that a particle position (x - s/2) has momentum p; 3 is the amplitude that a particle has the momentum p has position (x +s/2); (4) is the amplitude that a particle with position (x + s/2)

$$N := 60 \qquad i := 0 .. N \qquad x_i := -3 + \frac{6 \cdot i}{N} \qquad j := 0 .. N \qquad p_j := -5 + \frac{10 \cdot j}{N} \qquad Wigner_{i,j} := W_0\left(x_i, p_j\right)$$



Harmonic Oscillator Ground State Ψ(x,p) Position - Momentum 3-D Phase Space Probability Distribution

Wigner

In these phase-space calculations W(x,p) appears to behave like a classical probability function. By eliminating the need for differential operators, it seems to have removed some of the weirdness from quantum mechanics. The Wigner function, phase-space approach only temporarily hides the weirdness generated using a Schrödinger wave function.

To see how the weirdness is hidden we generate the Wigner function for the v = 2 harmonic oscillator state.

$$W_1(x,p) := \frac{1}{2\pi}\int_{-\infty}^{\infty} \Psi_1\left(x+\frac{s}{2}\right)\cdot\exp(i\cdot s\cdot p)\cdot\Psi_1\left(x-\frac{s}{2}\right) ds \text{ simplify}$$

$$W_1(x,p) := e^{-\left(x^2\right)-p^2}\cdot\frac{\left(2\cdot x^2+2\cdot p^2\right)-1}{\pi}$$

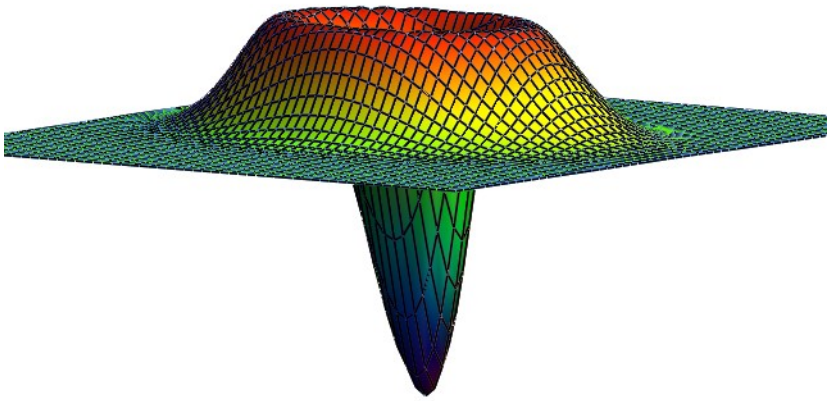
Next, it is demonstrate that the Wigner functions for the ground and excited harmonic oscillator states are orthogonal over phase space.

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} W_0(x,p)\cdot W_1(x,p)\,dx\,dp \to 0$$

This result indicates that W1(x,p) must be negative over some part of phase space, because the graph of W0(x,p) shows that it is positive for all values of position and momentum. To explore further we display the Wigner distribution for the v = 1 harmonic oscillator state.

$$Wigner_{i,j} := W_1\left(x_i, p_j\right)$$

Harmonic Oscillator v = 1 State
Ψ(x,p) Position - Momentum 3-D Phase Space
Probability Distribution



$Wigner, Wigner$

Given the quantum number this Mathcad file calculates the Wigner distribution function for the specified harmonic oscillator eigen state.

Quantum number: n:=2

Harmonic oscillator eigenstate:

$$n := 2 \qquad \Psi_2(x) := \frac{1}{\sqrt{2^n \cdot n! \cdot \sqrt{\pi}}} \cdot Her(n, x) \cdot exp\left(\frac{-x^2}{2}\right)$$

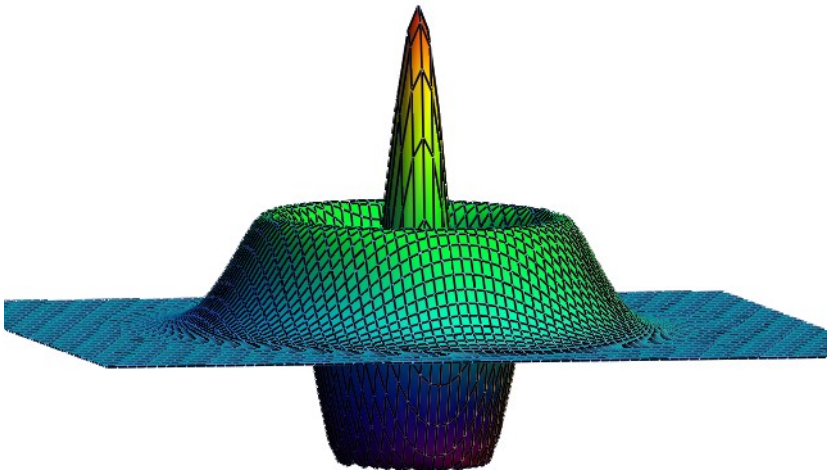
Calculate the Wigner distribution:

$$W_{n2}(x, p) := \frac{1}{\pi^{\frac{3}{2}}} \cdot \int_{-\infty}^{\infty} \Psi_2\left(x + \frac{s}{2}\right) \cdot exp(i \cdot s \cdot p) \cdot \Psi_2\left(x - \frac{s}{2}\right) ds$$

Display the Wigner distribution:

$$N := 80 \qquad i := 0..N \qquad x_i := -4 + \frac{8 \cdot i}{N} \qquad j := 0..N \qquad p_j := -5 + \frac{10 \cdot j}{N} \qquad Wigner2_{i,j} := W_{n2}\left(x_i, p_j\right)$$

Harmonic Oscillator v = 2 State
Ψ(x,p) Position - Momentum 3-D Phase Space
Probability Distribution



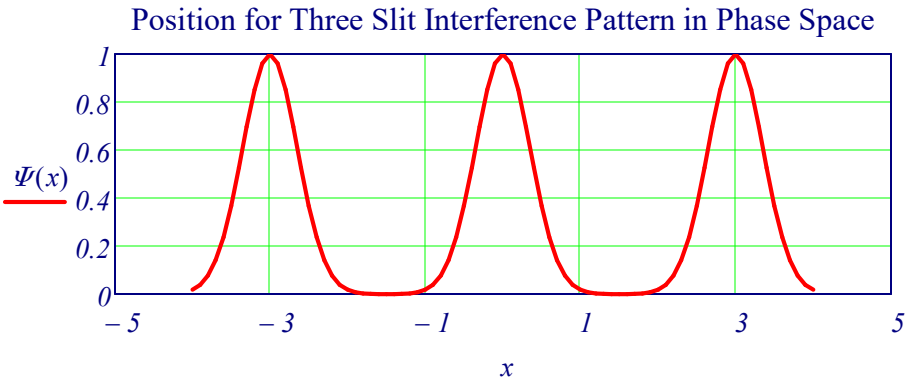
$Wigner_2, Wigner_2$

Basic QM Math: Wigner Quasiprobability Distribution for Triple-Slit Experiment

The quantum mechanical interpretation of the triple-slit experiment is that position is measured at the slit screen and momentum is measured at the detection screen. Position and momentum are conjugate observables connected by a Fourier transform and governed by the uncertainty principle. Knowing the slit screen geometry makes it possible to calculate the momentum distribution at the detection screen.

The slit-screen geometry and therefore the coordinate wavefunction is modeled as a superposition of three Gaussian functions.

$$\Psi(x) := exp\left[-4\cdot(x-3)^2\right] + exp\left(-4\cdot x^2\right) + exp\left[-4\cdot(x+3)^2\right]$$



The coordinate wavefunction is Fourier transformed into momentum space to yield the diffraction pattern. Note that this calculation is in agreement with the expectation that the number of minor maxima appearing between the major maxima is given by the number of slits minus 2.

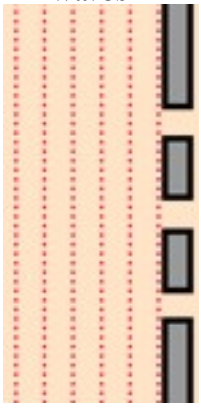
Momentum Expectation Function

$$\Phi(p) := \frac{1}{\sqrt{2\pi}}\cdot\int_{-\infty}^{\infty} exp(-i\cdot p\cdot x)\cdot\Psi(x)\,dx$$

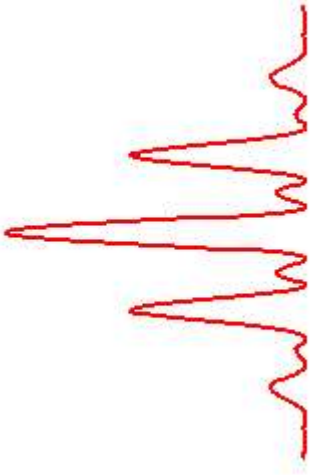
$$p := -6, -5.95 .. 6$$

Three Slit Demonstration for Momentum Φ(p)

Incident plane waves



Momentum Expectation *Φ(p)*

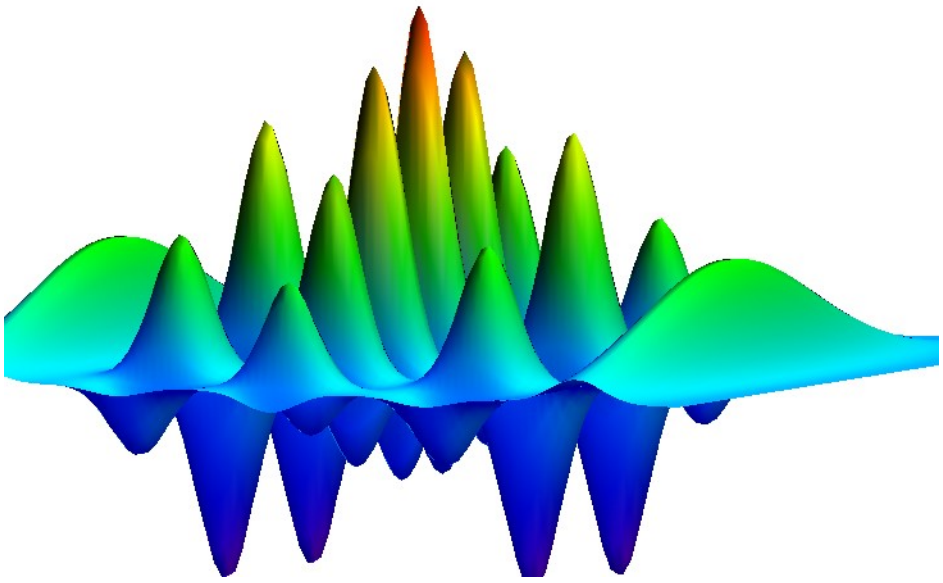


The Wigner function is a phase-space distribution that is obtained by the Fourier transform of either the coordinate or momentum wavefunction. We use the coordinate wavefunction.

$$W(x,p) := \frac{1}{\pi^{\frac{3}{2}}} \cdot \int_{-20}^{20} \Psi\left(x + \frac{s}{2}\right) \cdot exp(-i \cdot s \cdot p) \cdot \Psi\left(x - \frac{s}{2}\right) ds$$

$$N := 100 \qquad i := 0..N \qquad x_i := -4 + \frac{8 \cdot i}{N}$$

$$j := 0..N \qquad p_j := -6 + \frac{12 \cdot j}{N} \qquad Wigner3\phi_{i,j} := W\left(x_i, p_j\right)$$



$Wigner3\phi$

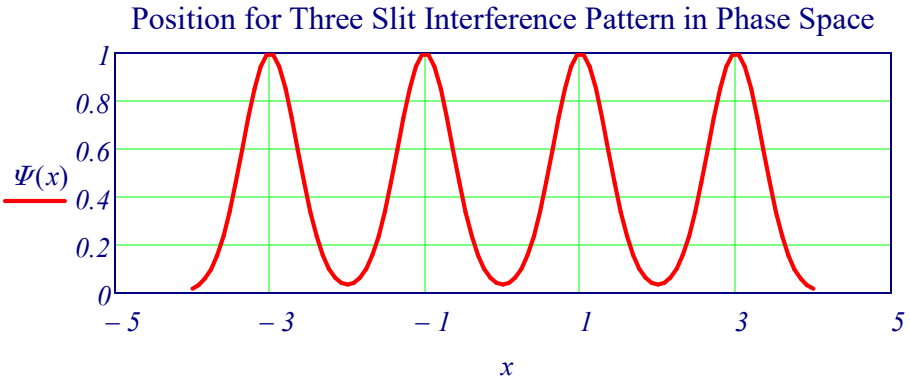
The Wigner distribution is frequently called a quasi-probability distribution because, as can be seen in the display above, it can have negative values. Integration of the Wigner function with respect to momentum recovers the coordinate wavefunction and integration with respect to position yields the momentum wavefunction.

Basic QM: Wigner Quasiprobability Distribution: Quadruple-Slit Experiment

The quantum mechanical interpretation of the triple-slit experiment is that position is measured at the slit screen and momentum is measured at the detection screen. Position and momentum are conjugate observables connected by a Fourier transform and governed by the uncertainty principle. Knowing the slit screen geometry makes it possible to calculate the momentum distribution at the detection screen.

The slit-screen geometry and therefore the coordinate wavefunction is modeled as a superposition of three Gaussian functions.

$$\Psi(x) := exp\left[-4\cdot(x-3)^2\right] + exp\left[-4\cdot(x-1)^2\right] + exp\left[-4\cdot(x+1)^2\right] + exp\left[-4\cdot(x+3)^2\right]$$

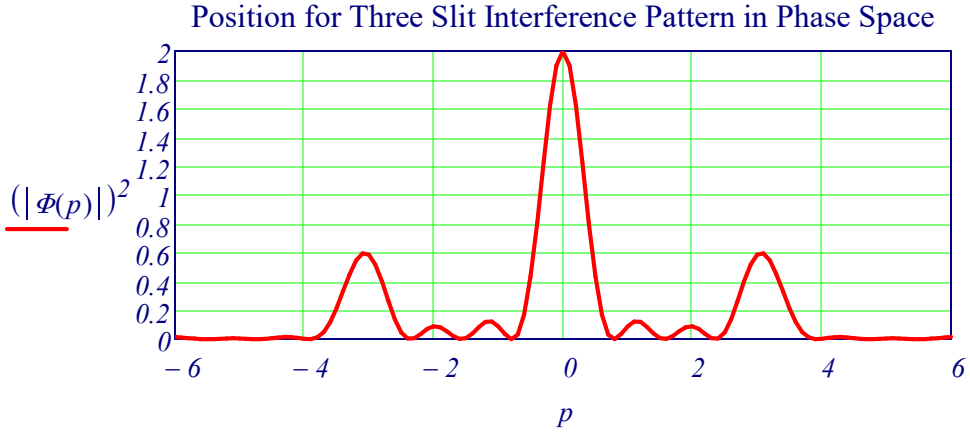


The coordinate wavefunction is Fourier transformed into momentum space to yield the diffraction pattern. Note that this calculation is in agreement with the expectation that the number of minor maxima appearing between the major maxima is given by the number of slits minus 2.

Momentum Expectation Function

$$\Phi(p) := \frac{1}{\sqrt{2\pi}}\cdot\int_{-6}^{6} exp(-i\cdot p\cdot x)\cdot\Psi(x)\,dx$$

$$p := -6, -5.9 .. 6$$

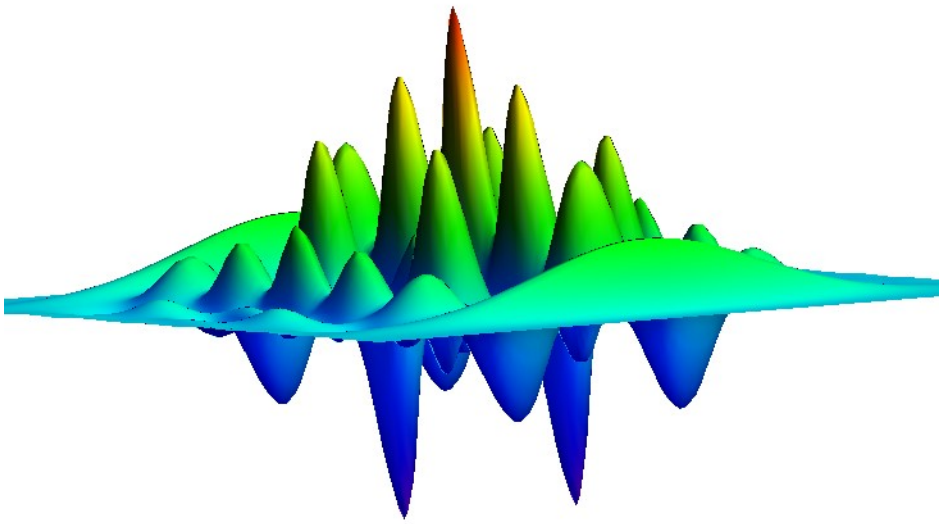


The coordinate wavefunction is Fourier transformed into momentum space to yield the diffraction pattern. Note that this calculation is in agreement with the expectation that the number of minor maxima appearing between the major maxima is given by the number of slits minus 2.

$$W(x,p) := \frac{1}{\pi^{\frac{3}{2}}} \cdot \int_{-20}^{20} \Psi\left(x + \frac{s}{2}\right) \cdot exp(i \cdot s \cdot p) \cdot \Psi\left(x - \frac{s}{2}\right) ds$$

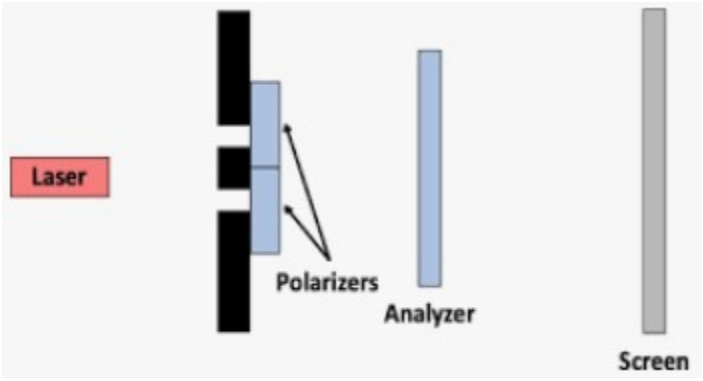
$$N := 100 \qquad i := 0..N \qquad x_i := -4 + \frac{8 \cdot i}{N}$$

$$j := 0..N \qquad p_j := -6 + \frac{12 \cdot j}{N} \qquad Wigner4\phi_{i,j} := W\left(x_i, p_j\right)$$



$Wigner4\phi$

XXIX. The Quantum Eraser



Assuming (initially) infinitesimally thin slits, the photon wave function at the slit screen is an entangled superposition of being at top slit with vertical polarization and bottom slit with polarization at an angle θ relative to the vertical. This entanglement provides which-way information if θ is not equal to 0 and, therefore, has an important effect on the diffraction pattern.

$$|\Psi\rangle = \frac{1}{\sqrt{2}}[|x_1\rangle\,|v\rangle + |x_2\rangle|\theta\rangle]$$

$$\langle p\phi|\Psi\rangle = \frac{1}{\sqrt{2}}[\langle p|x_1\rangle\,\langle\phi|v\rangle + \langle p|x_2\rangle\,\langle\phi|\theta\rangle]$$

This state is projected onto ϕ and p because a ϕ-oriented polarizer (eraser) precedes the detection screen and because a diffraction pattern is actually the momentum distribution of the scattered photons. In other words, position is measured at the slit screen and momentum is measured at the detection screen.

$$\langle p\phi|\Psi\rangle = \frac{1}{\sqrt{2}}[\langle p|x_1\rangle\cos(\phi) + \langle p|x_2\rangle\cos(\theta-\phi)]$$

The polarization brackets $\langle p\phi|\Psi\rangle$ (amplitudes) are easily shown to be the **above** trigonometric functions.

The position-momentum brackets <p|x> are the position eigenstates in the momentum representation and are given by:

$$\langle p|x\rangle = \frac{1}{\sqrt{2\pi\hbar}}\exp\left(-\frac{ipx}{\hbar}\right)$$

this allows us to write $\langle p\phi|\Psi\rangle = \frac{1}{\sqrt{2}}\left[\frac{1}{\sqrt{2\pi\hbar}}\exp\left(-\frac{ipx_1}{\hbar}\right)\cos(\phi) + \frac{1}{\sqrt{2\pi\hbar}}\exp\left(-\frac{ipx_2}{\hbar}\right)\cos(\theta-\phi)\right]$

Working in atomic units (h = 2π) and now assuming slits of finite width this expression becomes,

Slit positions: $x_1 := 1 \quad x_2 := 2$ Slit width: $\delta := 0.2$

$$\Psi(p,\theta,\phi) := \frac{1}{\sqrt{2}}\left(\int_{x_1-\frac{\delta}{2}}^{x_1+\frac{\delta}{2}} \frac{1}{\sqrt{2\cdot\pi}}\cdot exp(-i\cdot p\cdot x)\cdot\frac{1}{\sqrt{\delta}}\,dx\cdot cos(\phi) + \int_{x_2-\frac{\delta}{2}}^{x_2+\frac{\delta}{2}} \frac{1}{\sqrt{2\cdot\pi}}\cdot exp(-i\cdot p\cdot x)\cdot\frac{1}{\sqrt{\delta}}\,dx\cdot cos(\theta-\phi)\right)$$

Diffraction pattern as a histogram of photon arrivals at detection screen

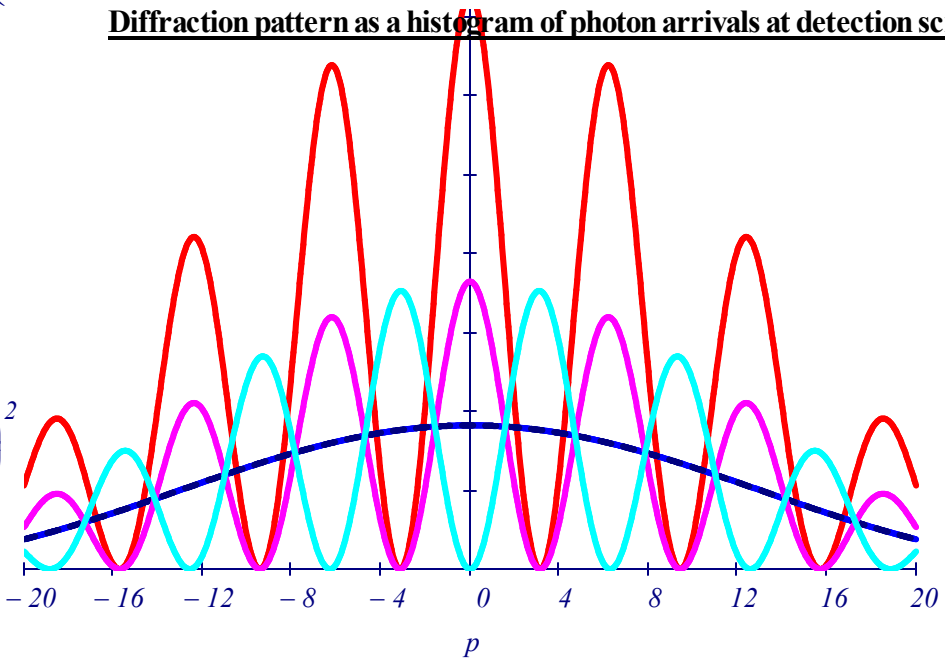
$(|\Psi(p,0,0)|)^2$

$\left(\left|\Psi\left(p,\frac{\pi}{2},0\right)\right|\right)^2$

$\left(\left|\Psi\left(p,\frac{\pi}{2},\frac{\pi}{2}\right)\right|\right)^2$

$\left(\left|\Psi\left(p,\frac{\pi}{2},\frac{\pi}{4}\right)\right|\right)^2$

$\left(\left|\Psi\left(p,\frac{\pi}{2},\frac{-\pi}{4}\right)\right|\right)^2$



Discussion of Results

The polarizer at top slit is always oriented vertically so only the orientations (θ and ϕ) of the other polarizers need to be specified.

The photons emerging from the slits are vertically polarized and encounter a vertical polarizer before the detection screen. This is the plot of $(|\Psi(p,0,0|))^2$. There is no which-way information in this experiment and 100% of the photons emerging from the vertically polarized slit screen reach the detection screen.

$$\int_{-\infty}^{\infty} (|\Psi(p,0,0)|)^2 dp \text{ float }, 3 \rightarrow 1.00$$

The crossed polarizers at the slit screen provide which-way information and the interference fringes disappear if the third polarizer is vertically or horizontally oriented. This is shown by the plots of $(|\Psi(p,\pi/2,0|))^2$ and $(|\Psi(p,\pi/2,\pi/2|))^2$. Furthermore, relative to the reference experiment, 50% of the photons reach the detection screen.

$$\int_{-\infty}^{\infty} \left(|\Psi\left(p,\frac{\pi}{2},0\right)|\right)^2 dp \text{ float }, 3 \rightarrow 0.500$$

$$\int_{-\infty}^{\infty} \left(|\Psi\left(p,\frac{\pi}{2},\frac{\pi}{2}\right)|\right)^2 dp \text{ float }, 3 \rightarrow 0.500$$

In the absence of the third polarizer, there is also no diffraction pattern but 100% of the photons reach the detection screen. $[\theta=\pi/2,\phi=\pi/4]$ and $[\theta=\pi/2,\phi=-\pi/4]$

The which-way information provided by the crossed polarizers at the slit screen is erased by diagonally and anti-diagonally oriented polarizers in front of the detection screen. This is shown by the plots of $(|\Psi(p,\pi/2,\pi/4)|)^2$ and $(|\Psi(p,\pi/2,-\pi/4)|)^2$

The reason the which-way information has been erased is that vertically and horizontally polarized photons emerging from slits 1 and 2 both have a 50% chance of passing the diagonally or anti-diagonally oriented third polarizer. Thus, it is impossible to determine the origin of a photon that passes the third polarizer and the interference fringes are restored. Again, for this experiment 50% of the photons reach the detection screen.

$$\int_{-\infty}^{\infty} \left(|\Psi\left(p,\frac{\pi}{2},\frac{\pi}{4}\right)|\right)^2 dp \text{ float }, 3 \rightarrow 0.500$$

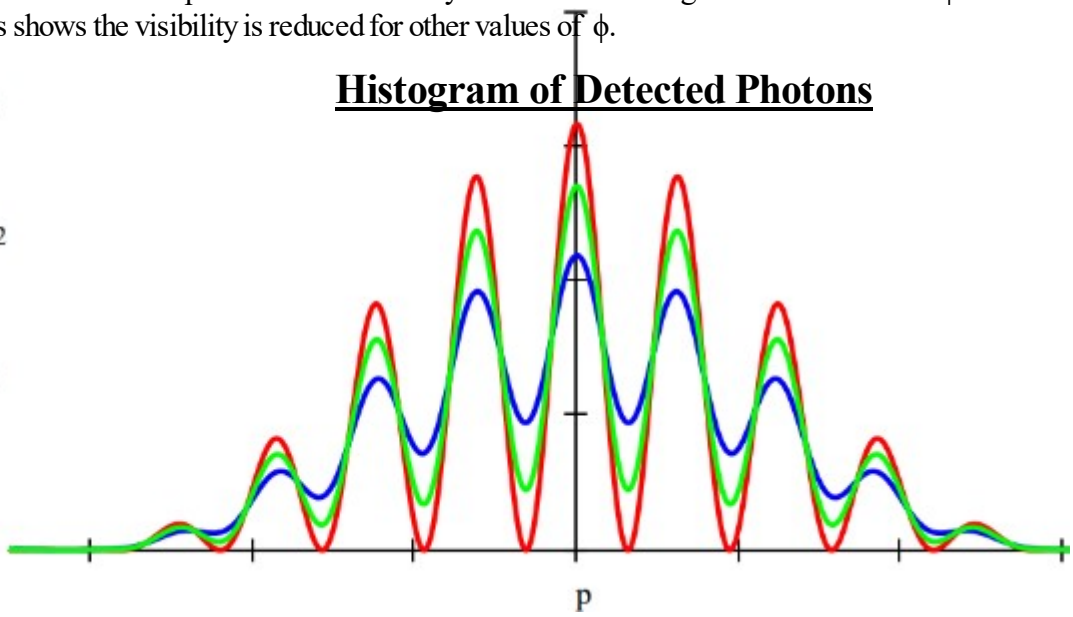
$$\int_{-\infty}^{\infty} \left(|\Psi\left(p,\frac{\pi}{2},-\frac{\pi}{4}\right)|\right)^2 dp \text{ float }, 3 \rightarrow 0.500$$

The shift in the interference fringes calculated for $(|\Psi(p,\pi/2,\pi/4)|)^2$ and $(|\Psi(p,\pi/2,-\pi/4)|)^2$ is observed in the Kwiat/Hillmer experiment. The visibility of the restored fringes is maximized for $\phi = \pm\pi 4$. As the figure belows shows the visibility is reduced for other values of ϕ.

$$\left(\left|\Psi\left(p,\frac{\pi}{2},\frac{\pi}{4}\right)\right|\right)^2$$

$$\left(\left|\Psi\left(p,\frac{\pi}{2},\frac{\pi}{16}\right)\right|\right)^2$$

$$\left(\left|\Psi\left(p,\frac{\pi}{2},\frac{\pi}{8}\right)\right|\right)^2$$



XXX. The Difference Between Fermions and Bosons: Math

Calculate the average separation, $|x_1 - x_2|$, for two fermions and two bosons in a 1D box of unit length.

$$n_1 := 1 \quad n_2 := 2 \quad \Psi(x) := \sqrt{2}\cdot\sin\left(n_1\cdot\pi\cdot x\right) \quad \Phi(x) := \sqrt{2}\cdot\sin\left(n_2\cdot\pi\cdot x\right)$$

Fermions have antisymmetric wave functions:

$$\Psi_f\left(x_1,x_2\right) := \frac{\Psi\left(x_1\right)\cdot\Phi\left(x_2\right) - \Psi\left(x_2\right)\cdot\Phi\left(x_1\right)}{\sqrt{2}}$$

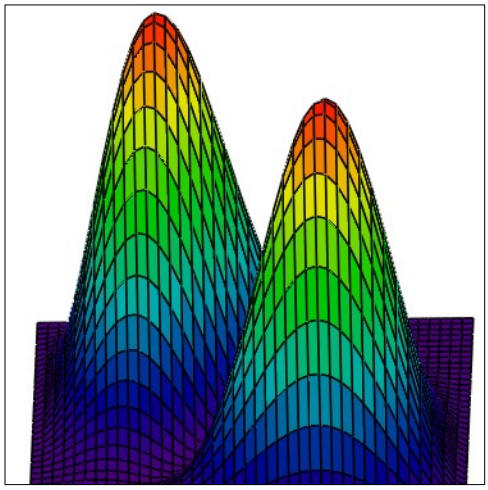
The average particle separation for indistinquishable fermions:

$$Separation\_Fermions := \int_0^1\int_0^1 \Psi_f\left(x_1,x_2\right)\cdot\left|x_1 - x_2\right|\cdot\Psi_f\left(x_1,x_2\right)\,dx_1\,dx_2 \qquad Separation\_Fermions = 0.383$$

The particles are correlated so as to keep them apart.

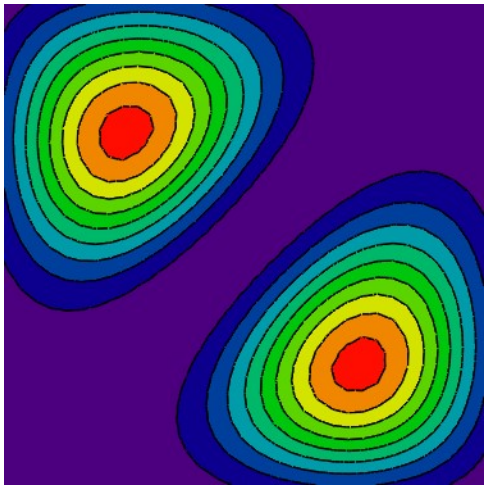
$$N := 40 \quad i := 0..N \quad x1_i := \frac{i}{N} \quad j := 0..N \quad x2_j := \frac{j}{N} \quad \Psi f_{i,j} := \Psi_f\left(x1_i,x2_j\right)^2$$

Fermion 3D Surface Plot



Ψ_f

Fermion Contour Plot



Ψ_f

Bosons have symmetric wave functions:

$$\Psi_b\left(x_1,x_2\right) := \frac{\Psi\left(x_1\right)\cdot\Phi\left(x_2\right) + \Psi\left(x_2\right)\cdot\Phi\left(x_1\right)}{\sqrt{2}}$$

Bosons Clump, Ferimons Separate

The average particle separation for indistinquishable bosons:

$$Separation\_Bosons := \int_0^1\int_0^1 \Psi_b\left(x_1,x_2\right)\cdot\left|x_1 - x_2\right|\cdot\Psi_b\left(x_1,x_2\right)\,dx_1\,dx_2$$

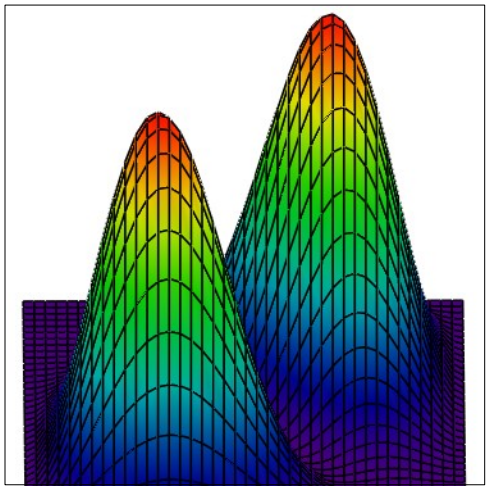
$Separation\_Fermions = 0.383$

$Separation\_Bosons = 0.157$

The particles are correlated so as to bring them closer together.

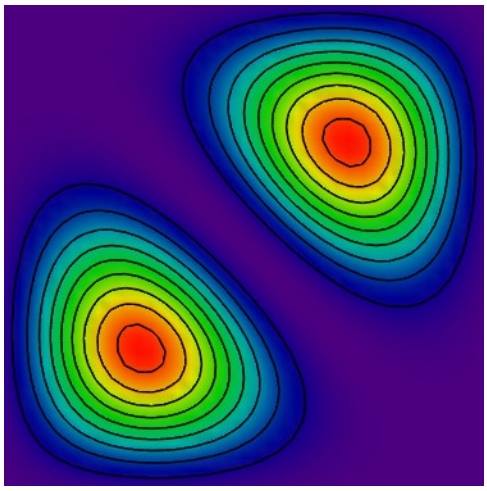
$N := 40 \quad i := 0..N \quad x1_i := \frac{i}{N} \quad j := 0..N \quad x2_j := \frac{j}{N} \quad \Psi b_{i,j} := \Psi b\left(x1_i, x2_j\right)^2$

Boson 3D Surface Plot



Ψ_b

Boson Contour Plot



Ψ_b

All fundamental particles (electrons, neutrons, protons, photons, etc.) are either bosons or fermions. Composite entities such as the elements also fall into these two categories. The fundamental distinction is spin: bosons have integer spin (0, 1, 2, ...) while fermions have half-integer spin (1/2, 3/2, ...).

The dramatic difference in behavior between bosons and fermions has led to a sociology of fundamental particles. Bosons are social and gregarious, while fermions are antisocial and aloof.

XXXI. Light Diffraction: Atomic Mask Diffraction Patterns: Math

The leading edge of semiconductors involve using more than 60 unique layers of lithography and accompanying steps. Extreme Ultraviolet, EUV, processing shrinks the laser wavelength size down to 13.5 nanometers. In order to create a single EUV mask, you have to first create the mask . At its very top is the mirror layer - a multi-layer Bragg reflector with 40-50 alternating layer pairs of molybdenum and silicon. The mask consists of transmission diffraction gratings. The diffracted coherent beams form an interference pattern which is recorded in the photoresist. The final pattern is formed from multiple interference patterns. Shown is the mask pattern result with just 5 atomic scatterers.

Establish mask geometry:

Number of Atoms: $A \quad A := 5$

$$R := 2 \qquad m_{\cdot} := 1 \,..\, A \qquad \Theta_{m_{\cdot}} := \frac{2 \cdot \pi \cdot m_{\cdot}}{A} \qquad x_{m_{\cdot}} := R \cdot \sin\left(\Theta_{m_{\cdot}}\right) \qquad y_{m_{\cdot}} := R \cdot \cos\left(\Theta_{m_{\cdot}}\right) \qquad d := .5$$

Calculate coordinate-space wave function:

$$\Psi_{\cdot\cdot}(xx, yy) := \frac{1}{\sqrt{A}} \cdot \sum_{m=1}^{A} if\left[\left[xx \geq \left(x_m - \frac{d}{2}\right)\right] \cdot \left[xx \leq \left(x_m + \frac{d}{2}\right)\right] \cdot \left[yy \geq \left(y_m - \frac{d}{2}\right)\right] \cdot \left[yy \leq \left(y_m + \frac{d}{2}\right)\right], 1, 0\right]$$

Fourier transform of position wave function into the momentum representation:

$$\Phi_{\cdot}\left(p_x, p_y\right) := \frac{1}{2 \cdot \pi \cdot \sqrt{A}} \cdot \sum_{m=1}^{A} \left(exp\left(-i \cdot p_x \cdot x_m\right) \cdot exp\left(-i \cdot p_y \cdot y_m\right)\right)$$

$$N := 100 \quad \Delta p := 10 \quad \Delta x := -3 \quad j := 0 \,..\, N \qquad xx_j := -\Delta x + \frac{2 \cdot \Delta x \cdot j}{N} \qquad p_{x_j} := -\Delta p + \frac{2 \cdot \Delta p \cdot j}{N}$$

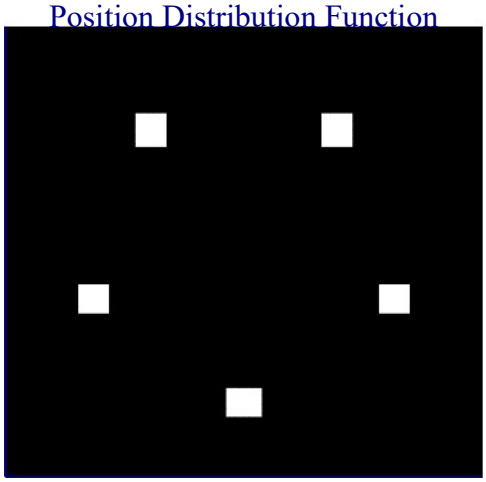
$$\Delta y := -3 \quad k := 0 \,..\, N \qquad yy_k := -\Delta y + \frac{2 \cdot \Delta y \cdot k}{N} \qquad p_{y_k} := -\Delta p + \frac{2 \cdot \Delta p \cdot k}{N}$$

Display slit pattern and diffraction pattern:

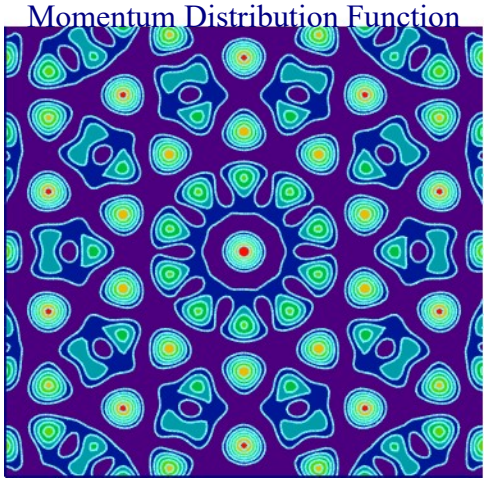
$$MaskPattern_{j,k} := \left(\left|\Psi_{\cdot\cdot}\left(xx_j, yy_k\right)\right|\right)^2$$

$$DiffractionPattern_{j,k} := \left(\left|\Phi_{\cdot}\left(p_{x_j}, p_{y_k}\right)\right|\right)^2$$

Position Distribution Function



Momentum Distribution Function



MaskPattern

DiffractionPattern

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Special Thanks to Dr. Frank Rioux and his Tutorials on *Physical_and_Theoretical_Chemistry*