Introduction to Quantum Information

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Preface

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     Information is something that can be encoded
 in the state of a physical system, and a computation
    is a task that can be performed with a physically
 realizable device. Therefore, since the physical world
is fundamentally quantum mechanical, the foundations
   of information theory and computer science should
        be sought in quantum physics. (John Preskill)
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With a background in high-energy Physics and in Computer Science, my interest in Quantum Information was evident after the *Simons Conference on New Trends in Quantum Computation* in 2010. Among some very introductory talks (and others not introductory at all), three were particularly very exciting: *Quantum Money from Knots* from Edward Farhi, *Quantum channel capacities* from Peter Shor, and *Philosophical and Practical aspects of Building a Quantum Computer*, from Michael Freedman.

There are many pedagogical resources covering different approaches in problems in quantum information and quantum computation. I've been studying those that I believe are appropriate to my interest, however I suggest the reader to go beyond what I present here. Moreover, these are notes made by a graduate student for graduate and undergraduate students, please take this in consideration when you read them. In the first part of these notes I put together the material from my studies, from [NC00], [PRES01], [KSV02], [MER05] and [STE06], and other related references. Then I keep track of up-to-date results on topological quantum computing, quantum information theory, and other related subjects.

Are Quantum Computers more Powerful than Classical Computers?

In these notes, we will learn that quantum computers differ from classical computation in several respects when it comes to the processing of the information. For example, we cannot read a quantum data without having the state becoming the measured value; from the *No Cloning Theorem*, an arbitrary state cannot be cloned; and the state may be in a superposition of basis values. However, the ability of manipulating quantum systems enables the perform of tasks that would not be

allowed in classical system (for example, factoring large numbers, or achieving dimensional sizes of physical devices that are comparable to quantum dimensions, such as the atoms), as well as the achievement of a new level of security of the information.

KSV's book, [KSV02], address to this question in a very solid way. First of all, in a quantum computer, it's possible to model an arbitrary quantum system in polynomially many steps (classical computer efficiency = polynomial time). Second, for problems such as factoring integers into prime number, Peter Shor in 1994, [SHO94], found a quantum algorithm which factorizes an n-digit integer in n^3 steps using abelian groups. The implementation of such solution would break the commonly used cryptography systems, such as RSA and ElGamal (whose relie completely on the factoring problem). Finally, for searches in an unsorted database, quantum computers locate one entry in $\sqrt{N}$ steps instead of N for classical computers.

These were arguments of a decade ago. Nowadays, one of the biggest challenges of quantum computing researchers is to understand/control the *decoherence*. This is the tendency of quantum systems to be disturbed, which leads to to errors caused by noises, and can be overcome by quantum error correction. In a quantum computer, errors are continuous, not just bit flips. Since measurement destroys the superposition, how do we know errors have occurred? Mike Freedman, Michael Larsen, Z. Wang and Kitaev showed in 2002,[FKLW02], that a topological quantum computer can simulate any computation of a standard quantum computer. Even considering that the simulation is approximate, given any accuracy, a braid can be found, and it will simulate the computation to that accuracy.

In the experimental point of view, there are already many approaches of realizing a quantum computer. The optical approach in trapping of ions, the use of nuclear magnetic resonance, the concept of quantum dots, the technology of superconductors devices (SQUIDS), among others, have been improved every day, with many new publications. A different (mathematical) approach, which is is also of my particular interest, is the use of *anyons* (basically, in two-dimensions, identical particles can pick up an arbitrary phase, and these excitations have been observed in the fractional quantum Hall effect) and their topological properties, [KIT97], [FRE98]. This gives rises to the *topological quantum information* (braiding particles with non-abelian statistics entangled) and I shall talk more about it in the end of this work.

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    "A two-dimensional quantum system with  anyonic excitations
 can be considered as a quantum computer. Unitary transformations
  can be performed by moving the excitations around each other.
Measurements can be performed by joining excitations in pairs and
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observing the result of fusion. Such computation is fault-tolerant by its physical nature." (A. Kitaev, 2008)

As a theoretical Physics student, on the one hand I'm interested on an entire class of problems related to quantum information theory, including aspects of classical and quantum cryptography, as well as the computational complexity theory and quantum algorithms. On the another hand, when it comes to the realization of quantum computers in the applications of topological theory for anyons, the discussion becomes also deep and interesting. As one example of this approach, Kitaev in 2008, [KIT97] stated the following problems:

1) It's is desirable to find other models with anyons which allow universal quantum computation. (S5 is quite unrealistic for physical implementation). Such models must be based on a more general algebraic structure rather than the quantum double of a group algebra. A general theory of anyons and topological quantum order is lacking.

2) It is also desirable to formulate and prove some theorem about existence and the number of local degrees of freedom. (It seems that the local degrees of freedom are a sign that anyons arise from a system with no symmetry in the Hamiltonian).

3) Finally, general understanding of dynamically created, or materialized symmetry is lacking. There one may find some insights for high energy physics. If we adopt a conjecture that the fundamental Hamiltonian or Lagrangian is not symmetric, we can probably infer some consequences about the particle spectrum.

In addition, the experimental achievements in this field are necessary to be mentioned, and I try to associate the discussions to the most interesting practical results. To reach all the proposed objectives, I will be keeping tracking of many of recent publications (and eventually briefly describe the papers) and real up-to-date problems as well.These notes are mostly for my own amusement, however I encourage the reader to send me any suggestion or comment.

Acknowledgment

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Marina von Steinkirch,
January of 2011.

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Part I

Fundamentals of Quantum Mechanics

Chapter 1

Quantum Mechanics

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Quantum Mechanics tells us WHAT
happens but does not tell us WHY
it happens and does not tell us either
HOW it happens nor HOW MUCH
it costs. (Josef Gruska)
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Everything starts with *quantum mechanics*. The following chapter represents the contend of a graduate course on the subject. Part of them are not necessarily relevant for treating quantum information problems. However, for completeness, I include them here. These chapter were based on the straightforward references [SAK93], [LL1981], and [GY68].

1.1 States

- The *states* of a quantum system at time t are given by a vector (ray) $|\alpha\rangle$ in a complex Hilbert space $\mathcal{H}$.
- The *observables* are given by hermitian operators, A, with complete set of eigenvectors (states). They are *hermitian*, i.e. $A = A^\dagger$. All eigenvalues a_i of A are real, and all states, $|\alpha\rangle$, are orthogonal.
- The probability of observing a is

$$\sum_j |\langle a_j|\alpha\rangle|^2 = \langle\alpha|A|\alpha\rangle$$

.

- Compatible observables commute, i.e. $[A, B] = AB - BA = 0$, and can be simultaneous diagonalized.

- For an observable A, with a state $|a\rangle$, the dispersion is

$$\langle \Delta A^2 \rangle = \langle A^2 \rangle - \langle A \rangle^2$$

.

- For two states α and β of the same system,

$$\text{tr } (|\beta\rangle\langle\alpha|) = \langle\alpha|\beta\rangle.$$

Proof. Let $|i\rangle$ be the complete basis vector of the Hilbert space such as $\sum_i |i\rangle\langle i| = \mathbf{1}$. From the definition of trace,

$$\text{tr } (|\beta\rangle\langle\alpha|) = \sum_i \langle i|\beta\rangle\langle\alpha|i\rangle = \langle\alpha|\Big(\sum_i |i\rangle\langle i\Big)|\beta\rangle = \langle\alpha|\beta\rangle.$$

□

- A skew-hermitian (anti-hermitian) operator is an operator satisfying $A^\dagger = -A$. A can have at most one real eigenvalue, which can be degenerate.

Proof. Let $|a\rangle$ the eigenstate of the operator A, then $\langle a|A|a\rangle = a$. Since $A = -A^\dagger$, $\langle a|A|a\rangle = -\langle a|A^\dagger|a\rangle = -a^* = a$. The only possible value is $a = 0$. □

- The equation $AB - BA = \mathbf{1}$ cannot be satisfied by any finite-dimensional matrices A, B.

Proof. We take the trace, $\text{tr } (AB) - \text{tr } (BA) = 0 \neq \text{tr}(\mathbf{1})$. □

- A hermitian (finite) matrix A can always be diagonalized by a unitary transformation. . A unitary operator, U, satisfies $U^*U = UU^* = \mathbf{1}$. In the eigenvalue equation $U|\lambda\rangle = \lambda|\lambda\rangle$, if U is unitary, $\lambda = e^{i\theta}$, with θ real.

Proof. Taking the complex conjugate of the eigenvalue equation,

$$(U|\lambda\rangle)^\dagger = \langle\lambda|U^\dagger = \langle\lambda|\lambda^*$$

. Sandwiching it with $|\lambda\rangle$, $\langle\lambda|U^\dagger U|\lambda\rangle = 1 = |\lambda|^2$. □

- If both $|\mu\rangle$, $|\lambda\rangle$ are eigenstates of U, supposing $\lambda \neq \mu$, then $\langle\mu|\lambda\rangle = 0$.

  Proof. Writing $U|\lambda\rangle = \lambda|\lambda\rangle$ and $U|\mu\rangle = \mu|\mu\rangle$, taking the complex conjugate of the second and subtracting them, $0 = \langle\mu|U^\dagger U - \mathbf{1}|\lambda\rangle = (\mu^*\lambda - \mathbf{1})\langle\mu|\lambda\rangle$.

  Since U is unitary $\mu^*\mu = 1$. Inserting one, $0 = \mu^*(\lambda - \mu)\langle\mu|\lambda\rangle$. The initial assumption was $\langle\mu|\lambda\rangle \neq 0$, following that $\mu = \lambda$. □

- Any 2×2 matrix X can be expanded into the *Pauli matrices* ,

  $$X = a_\mu \sigma^\mu,$$

  where $\mu = 0, 1, 2, 3$[1] and a_μ are complex numbers. For any X,

  $$a_\mu = \frac{1}{2}\mathrm{tr}(X\sigma_\mu).$$

- If X is a hermitian matrix, all a_μ are real.

  Proof. If X is hermitian, $X^\dagger X$, therefore $\sum_i a_i^* \sigma_i^\dagger = \sum_i a_i \sigma_i$. The Pauli matrices are all hermitian, therefore $\sum_i (a_i - a_i^*) = 0$. Since the Pauli matrices are a set of linearly independent matrices, in $a_i = a_i^*$. □

- The time evolution of a state $|\alpha\rangle$ is $e^{-\frac{i}{\hbar}E_\alpha t}$, where E_α is the eigenvalue. Therefore the time evolution of a state can be written as $|\psi(t)\rangle = e^{-i\hat{H}t/\hbar}|\psi(t=0)\rangle$, found from the Schroedinger equation

  $$i\hbar\frac{\partial}{\partial t}|\psi\rangle = \hat{H}|\psi\rangle,$$

  with some initial condition $|\psi(t=0)\rangle$.

- In an alternative picture, the *Heisenberg equation of motion* is given by

  $$i\hbar\frac{\partial\hat{O}}{\partial t} = [O, \hat{H}](t),$$

  where $O(t) = e^{iHt/\hbar}Oe^{-iHt/\hbar}$.

[1] Einstein summation convention: $A_\mu B^\mu = \sum_\mu A \cdot B$.

An Example of Linear Algebra in Quantum Mechanics

Let us consider two matrices

$$A = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{pmatrix}, B = \begin{pmatrix} 2 & 1 & 1 \\ 1 & 0 & -1 \\ 1 & -1 & 2 \end{pmatrix}.$$

They commute, $[A, B] = 0$, therefore they have the same eigenvectors(states). To find these states and the eigenvalues (spectrum), we use the characteristic equations $\det(A - \lambda_A) = 0$ and $\det(B - \lambda_B) = 0$, which results that A is degenerate, therefore we calculate the eigenstate from the non-degenerate B. Let us say that the final eigenstates are u_1, u_2, u_3.

It is possible to find a unitary transformation which simultaneously diagonalizes A and B such that $U^\dagger AU$ and $U^\dagger BU$ are diagonal. . This matrix is given by $U = (u_1, u_2, u_3)$.

Proof.

$$U^\dagger BU = \begin{pmatrix} u_1^\dagger \\ u_2^\dagger \\ u_3^\dagger \end{pmatrix} (\lambda_{B1}u_1, \lambda_{B2}u_2, \lambda_{B3}u_3) = \begin{pmatrix} \lambda_{B1} & 0 & 0 \\ 0 & \lambda_{B2} & 0 \\ 0 & 0 & \lambda_{B3} \end{pmatrix}$$

□

1.2 Schroedinger Equation and Single-Particle Potentials

1.2.1 Schroedinger Equation

The Schroedinger equation is an equation that describes how the quantum state of a physical system changes in time. Given a Hamiltonian operator of the system, H, the equation is

$$H\Psi = E\Psi \tag{1.2.1}$$

$$H\Psi = i\hbar\frac{\partial}{\partial t}\Psi \tag{1.2.2}$$

where is the eigenvalues (energy) and Ψ the eigenstates (wavefunction that solves the equation). In the *braket* formalism,

$$H|\alpha\rangle = a|\alpha\rangle. \tag{1.2.3}$$

Fir a single particle in a potential, $V(\vec{x})$, in 3+1-dimensions, the Hamiltonian is in the form

$$H = \frac{p^2}{2m} + V(\vec{x}) = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x}), \tag{1.2.4}$$

where $p = -i\hbar\nabla$.

1.2.2 Infinite Potential Well

The unidimensional infinite potential well is

$$V(x) = \begin{cases} 0, & 0 < x < L \\ \infty, & \text{otherwise} \end{cases}$$

Solving the Schroedinger equation [SAK93], the eigenvalues (energies) and eigenstates (wavefunctions) are

$$E_n = \frac{\pi\hbar^2 n^2}{2ma^2},$$
$$\Psi_n = \sqrt{\frac{2}{a}}\sin(\frac{n\pi x}{a}).$$

The force exerted by this particle on the potential wall can be estimated,

$$F = -\frac{\partial\langle E\rangle}{\partial(2a)}.$$

1.2.3 Finite Potential Well

The unidimensional infinite potential well with boundaries at $a, -a$ is

$$V(x) = \begin{cases} 0, & \text{inside}, -a < x < a; \\ E - V, & \text{outside}, x > a, x < -a; \end{cases}$$

Solving the Schroedinger equation [SAK93], it results in transcendental equations

$$\Psi(x) = \begin{cases} A\sin kx + B\cos kx, & -a < x < a; \\ Ce^{xk'}, & a < x; \\ Ce^{-xk'} & x < -a; \end{cases}$$

1.2.4 Delta Potential

The attractive delta potential can be written as

$$V(x) = -\frac{\hbar^2 \lambda}{2ma}\delta(x).$$

Resulting in the following equation to be solved is:

$$\frac{d^2u(x)}{dx^2} - k^2u(x) = -\frac{\lambda}{a}\delta(x)u(x),$$
$$\text{with } k^2 = \frac{2m|E|}{\hbar^2}.$$

The solution, everywhere except at $x = 0$, must satisfy the equation:

$$\frac{d^2u}{dx^2} - k^2u^2 = 0,$$

and at $x \to \pm\infty$ we have:

$$u(x) = e^{-kx}, x > 0,$$
$$u(x) = e^{kx}, x < 0.$$

Imposing boundary conditions,

$$-k - k = -\frac{\lambda}{a}.$$

1.2.5 Double Delta Potential Well

In the case of the double delta potential, the equation to be solved is

$$\frac{2m}{\hbar^2}V(x) = -\frac{\lambda}{a}(\delta(x-a) + \delta(x+a))$$

The solutions are **even** (always a single bound state), and **odd** (at most one bound state).

1.2.6 Harmonic Oscillator Potential

The unidimensional harmonic oscillator potential is

$$V(x) = \frac{1}{2}m\omega^2 x^2,$$

where ω is the angular frequency of the oscillator. The eigenvalues (energies) are

$$E_n = (n + \frac{1}{2})\hbar\omega.$$

We can represent the states in term of the *lowering* and *raising operators* (or creation and annihilation operators), respectively, $\hat{a}, \hat{a}^\dagger$. In terms of position $\hat{x}$ and momentum $\hat{p}$,

$$\hat{a} = \sqrt{\frac{\mu\omega}{2\hbar}}\Big(\hat{x} + \frac{i\hat{p}}{\mu\omega}\Big),$$
$$\hat{a}^\dagger = \sqrt{\frac{\mu\omega}{2\hbar}}\Big(\hat{x} - \frac{i\hat{p}}{\mu\omega}\Big),$$

where $[\hat{x}, \hat{p}] = i\hbar$ and $[\hat{a}, \hat{a}^\dagger] = 1$. Inverting these equations,

$$\hat{x} = \sqrt{\frac{\hbar}{2\mu\omega}}\Big(\hat{a} + \hat{a}^\dagger\Big),$$
$$\hat{p} = -i\sqrt{\frac{\hbar\mu\omega}{2}}\Big(\hat{a} - \hat{a}^\dagger\Big).$$

For many states,

$$\langle n|\hat{x}|n'\rangle \;=\; \sqrt{\frac{\hbar}{2m\omega}}\Big(\sqrt{n'}\delta_{n,n'-1} + \sqrt{n}\delta_{n',n+1}\Big).$$

Example: A linear harmonic oscillator in its ground state is exposed to a spatially constant force. At time $t = 0$, the force is suddenly removed. Compute the transition probabilities to the excited states.

When $t < 0$, the Hamiltonian is

$$H = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2} - Fx.$$

We rewrite the Hamiltonian as

$$H = \frac{p^2}{2m} + \frac{m\omega^2}{2}\Big(x - \frac{F}{m\omega^2}\Big)^2 - \frac{F^2}{2m\omega^2},$$

and introduce the change of variables $\xi = x/\lambda$, where $\lambda = \sqrt{\hbar/m\omega}$. The stationary Schroedinger equation becomes

$$-\frac{1}{2}\psi_f''(\xi) + \frac{1}{2}(\xi - f)^2\psi_f(\xi) = \epsilon_f,$$

where $f = \lambda F/\hbar\omega$, and $E_f/\hbar\omega - f^2/2$. The solutions are given by the *Hermite polynomials* , H_n,

$$\psi_{f_n}(\xi) = \frac{1}{\pi^{1/4}}\frac{1}{\sqrt{2^n n!}} e^{-\frac{(\xi+f)^2}{2}} H_n(\xi + f).$$

In the ground state, $n = 0$, $H_0 = 1$ resulting $\psi_{f_0}(\xi) = \frac{1}{\pi^{1/4}} e^{-\frac{(\xi+f)^2}{2}}$. Setting $f = 0$, the wavefunctions are

$$\psi_n(\xi) = \frac{1}{\pi^{1/4}}\frac{1}{\sqrt{2^n n!}} e^{-\frac{\epsilon^2}{2}} H_n(\xi). \tag{1.2.5}$$

The transition amplitude is giving by this two wavefunctions

$$\langle \psi_{f_0} | \psi \rangle = \int d\xi \psi_{f_0}(\xi)\psi_n(\xi).$$

Example: The Oscillator+Infinite Well Potential.

Let us find the eigenstates and eigenenergies of a particle in the potential

$$V(x) = \begin{cases} \frac{m\omega^2 x^2}{2}, & x > 0 \\ +\infty, & x < 0 \end{cases}$$

The ground state of the harmonic oscillator is given by equation (1.2.5),

$$\psi_0(\xi) = \frac{1}{\pi^{1/4}} e^{-\frac{\xi^2}{2}}.$$

We now put a barrier in the middle, representing the infinite potential well. The eigenstates will have to vanish at $\xi = 0$, resulting in wavefunctions with only odd Hermite polynomials, therefore, the eigenstates are

$$\psi_n(\xi) = \frac{1}{\pi^{1/4}}\sqrt{\frac{2}{2^{2n+1}(2n+1)!}} e^{-\frac{\xi^2}{2}} H_{2n+1}(\xi),$$

where the extra factor of $\sqrt{2}$ is the normalization on $\xi \in [0, \infty)$. The eigenstates are

$$E_n = \hbar\omega(2n + \frac{3}{2}).$$

1.2.7 Charged Particle in Magnetic Field

The Hamiltonian of a charged particle in a uniform magnetic field B is given by

$$H = \frac{1}{2m}\Big(\vec{p} - \frac{e}{c}\vec{A}\Big) = \frac{m\vec{v}^2}{2},$$

where $\partial_x A_y - \partial_y A_z = B$. A classical particle moves according to $v_i = \pm\omega_B(x_i - x_{i0})$, where $\omega_B = eB/mc$ is the cyclotron frequency.

Example: Hamiltonian of a Particle on a Ring in the Presence of a Magnetic Flux.

A Hamiltonian of a particle on a ring of radius R in a magnetic flux has a form of

$$H = \frac{L^2}{2mR^2},$$

where L is an operator of an angular momentum $L = -i\hbar\partial_\phi - \frac{e}{c}\frac{A_\phi}{R}$, A_ϕ the component of the vector potential along the ring. We can choose the gauge in which $A_\phi = \text{const}$.

The flux is given by

$$\Phi = \int d\vec{S}\cdot\vec{B} = \oint d\vec{l}\cdot\vec{A} = 2\pi R A_\phi.$$

The Hamiltonian can be write as

$$H = -\frac{\hbar^2}{2MR^2}\Big(\partial_\phi - i\frac{\Phi}{\Phi_0}\Big)^2,$$

where $\Phi_0 = 2\phi\hbar c/e$. The eigenvalues will be

$$E = \frac{\hbar^2}{2MR}\Big(M - \frac{\Phi}{\Phi_0}\Big)^2,$$

Using the boundary condition $\psi(\phi) = \psi(\phi + 2\pi)$, M must be an integer, $M = 0, \pm1, \pm2....$ The eigenstates are then

$$\psi_M(\phi) = \frac{1}{\sqrt{2\pi}}e^{iM\phi}.$$

Example: Spectra of a Particle in $\vec{B}$ and in a Harmonic Potential.

Let us analyze the problem of finding the ground state wavefunction and energy of a particle in a constant magnetic field B and in a strong external harmonic potential. The Hamiltonian is given by

$$H = \frac{1}{2m}\Big(-i\hbar\nabla - \frac{e}{c}\vec{A}\Big)^2 + \frac{m\omega_0^2}{2}(x^2+y^2).$$

Without magnetic field, the angular momentum of the ground state is zero and this will be not changed in a a magnetic field as the harmonic potential becomes strong. To find the solutions of this Hamiltonian, we first choose the radial gauge $A_x = -By/2$ and $A_y = Bx/2$ and rewrite it in polar coordinates,

$$H = -\frac{\hbar^2}{2m}\Big(\frac{1}{r}\partial_r r\partial_r + \frac{1}{r^2}\partial_\phi^2\Big) + i\frac{\hbar^2}{2m}\frac{eB}{\hbar c}\partial_\phi + \frac{m}{2}\Big(\omega_0^2 + \frac{\omega_B^2}{4}\Big)r^2,$$

where $\omega_B = eB/mc$. We separate variables and we get solutions in the form $e^{iL}\phi\psi_L(r)$. In the ground state of the oscillator, $L = 0$ and

$$H_{L=0} = -\frac{\hbar^2}{2m}\frac{1}{r}\partial_r r\partial_r + \frac{m}{2}\Big(\omega_0^2 + \frac{\omega_B^2}{4}\Big)r^2.$$

This is the Hamiltonian of the 2D oscillator with the frequency $\omega = \sqrt{\omega_0^2 + \omega_B^2/4}$. The ground state energy is $E_0 = \hbar\omega$ and the wavefunction of the ground state $\psi = \frac{1}{\sqrt{2\pi\lambda^2}}e^{-\frac{r^2}{2\lambda^2}}$, where $\frac{1}{\lambda^2} = \frac{m\omega}{\hbar}$.

1.2.8 Integer Quantum Hall Effect

Let us work in a simple toy model that gives some intuition about the *Integer Quantum Hall Effect* (IQHE)[2]. Let us consider a electron gas confined to the 2D xy-plane and neglect the interaction between electrons. The Hamiltonian of a particle is

$$H = \frac{1}{2m}\Big(-i\hbar\nabla - \frac{e}{c}\vec{A}\Big)^2 + V(x,y),$$

where $V(x,y)$ is an electrostatic confining potential and we can take it to be the one-dimensional harmonic oscillator $V = \frac{1}{2}m\omega_0^2 y^2$.

[2]Exercise proposed by Prof. Abanov, [ABA09]

For the constant magnetic field B we can use the Landau gauge $A_x = -By, A_y = 0$, and separate the variables $\psi(x,y) = \psi_k(y)e^{-ikx}$ to write down the stationary Schroedinger equation for $\psi_k(y)$. We introduce the cyclotron frequency $\omega_B = \frac{eB}{mc}$ and the magnetic length $l = \sqrt{\frac{\hbar c}{eB}}$ and the Hamiltonian becomes

$$H_k = \frac{\hbar^2}{2m}(-i\partial_y)^2 + \frac{m\omega_B^2}{2}(y - kl^2)^2 + \frac{m\omega_0^2}{2}y^2,$$

where the Schroedinger equation is $H_k\psi_k(y) = E\psi_k$.

We can identify this Hamiltonian with the harmonic oscillator for each k, with oscillator frequency $\sqrt{\omega_B^2 + \omega_0^2}$, rewriting as

$$H_k = \frac{\hbar^2}{2m}(-\partial_y)^2 + \frac{m(\omega_B^2 + \omega_0^2)}{2}(y - y_k)2 + \frac{m}{2}\frac{\omega_B^2\omega_0^2}{\omega_B^2 + \omega_0^2}k^2l^4,$$

where $y_k = \frac{\omega_B^2}{\omega_B^2+\omega_0^2}kl^2$. The energy levels are

$$E_{k,n} = \hbar\sqrt{\omega_B^2 + \omega_0^2}\Big(n + \frac{1}{2}\Big) + \frac{m}{2}\frac{\omega_B^2\omega_0^2}{\omega_B^2 + \omega_0^2}k_0^2l^4.$$

The levels at some n belong to the same *Landau level*. We can continue our analysis assuming that the chemical potential μ is such that the Landau levels with $n > 0$ are empty, i.e. $E_{n,k} > \mu$ for $n > 0$. The only occupied states are the ones with $n = 0$. The filled condition are then given by $E_{n,k} = \mu$ and gives $-k_0 < k < k_0$(the maximal and minimal values of k of the occupied levels), with

$$\mu = \frac{1}{2}\hbar\sqrt{\omega_B^2 + \omega_0^2} + \frac{m}{2}\frac{\omega_B^2\omega_0^2}{\omega_B^2 + \omega_0^2}k_0^2l^4.$$

The oscillator states are at $y = y_k$ and the filled states have their centers (The positions of the occupied levels) in $-y_0 < y < y_0$, with $y_0 = \frac{\omega_B^2}{\omega_B^2+\omega_0^2}k_0l^4$, at a defined μ.

Finally, the states with maximal and minimal k are the edge states of IQHE. These edge states have momentum $\hbar k_0$ and energy $E_{k_0,n=0}$. The velocity of corresponding boundary excitations are obtained by differentiating the energy over the momentum,

$$v_0 = \frac{1}{\hbar}\frac{\partial E_{k,n=0}}{\partial k}\Big|_{k=k_0} = c\frac{E_0}{B},$$

where E_0 is the confining electric field at the boundary and the result represents the drift velocity in crossed magnetic and electric fields.

1.2.9 The Tight Binding Model on 1D Lattice

The Hamiltonian for the tight binding model on unidimensional lattice can be written as

$$H = -t\sum_{n=1}^{N}\Big(|n+1\rangle\langle n| + |n\rangle\langle n+1|\Big).$$

It is convenient to make use of the states

$$|p\rangle = \frac{1}{\sqrt{N}}\sum_{n=1}^{N} e^{ipn}|n\rangle,$$
$$|n\rangle = \sum_{k} e^{-p_k n}|p_k\rangle,$$

which are Fourier transform of each other. For a complete set of states $\sum_k |p_k\rangle\langle p_k| = \mathbf{1}$,

$$|n\rangle = \sum_k |p_k\rangle\langle p_k|n\rangle = \sum_k e^{-ip_k n}|p_k\rangle.$$

The spectrum will be defined by

$$E_k = -2t\cos\Big(\frac{2\pi k}{N}\Big), \tag{1.2.6}$$

with $k = 0, 1, ..N-1$.

Translation Operator

For a N-dimensional Hilbert space with orthonormal basis $|n\rangle, n = 1, 2, ..., N$ the translation operator is

$$T = \sum_{n=1}^{N} |n+1\rangle\langle n|,$$

which is a unitary operator.

Proof. $TT^\dagger = \sum_{n,m} |n+1\rangle\langle n|m\rangle\langle m+1| = \sum_n |n+1\rangle\langle n+1| = 1$, where we used $\langle n|m\rangle = \delta_{nm}$. □

Other propriety of T is that it commutes with the previous Hamiltonian, $[H, T] = 0$ (which can be proved writing $H = -(T+T^\dagger)$), and that $T^N = -1$.

Proof. $T^N = \left(\sum_n |n\rangle\langle n+1|\right)^N = |n_1\rangle\langle n_1+1|n_2\rangle\langle n_2+1|...|n_N\rangle\langle n_N+1|$. Since $n_i = n_{i-1} + 1$, all factors in the middle become one, and we have $T^N = \sum_n |n\rangle\langle n+N| = \sum_n |n\rangle\langle n| = 1$, where we use have used the periodicity $|n+N\rangle = |n\rangle$. □

Tight Binding Model on a Finite Bethe Lattice

Let us consider a tight binding model on a finite Bethe lattice, with coordination number three and with only two generations of sites. This is given by the one-particle Hamiltonian

$$H = t \sum_{m,n} |m\rangle\langle n|.$$

where t is the constant called hopping amplitude and the sum is over all pairs $\rangle m, n\langle$ of sites connected to each other by an edge. If for example we put two noninteraction spinless fermion on the Bethe lattice, the energies of the states are given by the sum of the energies of occupied levels.

1.3 Spin-$\frac{1}{2}$ Systems and Angular Momentum

1.3.1 Pauli Matrices

The four Pauli matrices are

$$\sigma_0 = \mathbf{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \sigma_x = \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

$$\sigma_y = \sigma_2 \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_3 = \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

They have the following properties,

$$[\sigma_i, \sigma_j] = 2i\sigma_k \epsilon^{ijk}, \tag{1.3.1}$$
$$\det \sigma_i = -1, \tag{1.3.2}$$
$$\text{tr } \sigma_i = 0, \tag{1.3.3}$$
$$(\sigma_i)^2 = 1, \tag{1.3.4}$$
$$(\sigma \cdot a)(\sigma \cdot a) = (a)^2 \cdot 1, \tag{1.3.5}$$
$$(\sigma \cdot a)(\sigma \cdot b) = (a.b) \cdot 1 + i\sigma(a \times b), \tag{1.3.6}$$
$$(\sigma \cdot n)^k = 1, \text{ if k is even}, \tag{1.3.7}$$
$$(\sigma.n)^k = (\sigma.n), \text{ if k is odd}, \tag{1.3.8}$$
$$\sigma_i \sigma_j = \frac{1}{2}\{\sigma_i, \sigma_j\} + \frac{1}{2}[\sigma_i, \sigma_j] = \delta_{ij} + i\epsilon_{ijk}\sigma_k, \tag{1.3.9}$$
$$\text{tr } (a \cdot \sigma)(b \cdot \sigma)(c \cdot \sigma) = a_i \cdot b_j \cdot c_k \text{ tr } (\sigma_i \sigma_j \sigma_k) = 2ia(b \times c), \tag{1.3.10}$$
$$e^{i\theta\vec{\sigma}\cdot\vec{n}} = \cos(\theta) + i\vec{\sigma} \cdot \vec{n} \sin(\theta), \tag{1.3.11}$$
$$(\vec{\sigma}^1 + \vec{\sigma}^2)^2 = \sigma^2 \otimes 1 + 1 \otimes \sigma^2 + 2(\sigma \otimes \sigma). \tag{1.3.12}$$

The spectrum and eigenvectors of these matrices are find by the eigenvalue equation $\det(\sigma_i - \lambda_i) = 0$. We shall find the eigenvalues: $\lambda_1 = \lambda_2 = \lambda_3 = \pm 1$. The eigenvectors (eigenstates) are found by

$$\sigma_i \begin{pmatrix} a \\ b \end{pmatrix} = \pm \begin{pmatrix} a \\ b \end{pmatrix}.$$

Resulting

$$|\sigma_1\rangle = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \text{ and } |\sigma_1\rangle = \begin{pmatrix} 1 \\ -1 \end{pmatrix},$$

$$|\sigma_2\rangle = \begin{pmatrix} 1 \\ i \end{pmatrix} \text{ and } |\sigma_2\rangle = \begin{pmatrix} 1 \\ -i \end{pmatrix},$$

$$|\sigma_3\rangle = |+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ and } |\sigma_3\rangle = |-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

Example: Calculating the Exponential of Matrices using the Pauli Basis.

Let us calculate

$$A = e^M = exp \begin{pmatrix} 3 & 4 \\ 2 & 1 \end{pmatrix}.$$

We divide A in a traceless part and the rest by subtracting a term proportional to the unit,

$$M = 2 \cdot 1 + \begin{pmatrix} 1 & 4 \\ 2 & -1 \end{pmatrix} = 2 \cdot 1 + M'.$$

We then verify that $M'^2 \propto 1 = 1 \cdot 9$ and we can write $M'^{2n} = 9^n \cdot 1$ and $M'^{2n+1} = 9^n \cdot M'$. We can plug this result in the expansion of the exponential,

$$e^M = e^2 e^{M'} = e^2 \sum_n \Big(\frac{1}{(2n)!} M'^{2n} + \frac{1}{(2n+1)!} M'^{2n+1} \Big) = e^2 \Big(1 \cosh 3 + \frac{M'}{3} \sinh 3 \Big).$$

1.3.2 Spin-$\frac{1}{2}$ Systems

A system of a particle with spin-$\frac{1}{2}$ (fermion, such as an electron) can be measured by the following spin operators in function of the Pauli matrices,

$$\begin{aligned} S_x &= \frac{\hbar}{2}\sigma_x = \frac{\hbar}{2}\Big(|+\rangle\langle -| + |-\rangle\langle +| \Big), \\ S_y &= \frac{\hbar}{2}\sigma_y = \frac{i\hbar}{2}\Big(-|+\rangle\langle -| + |-\rangle\langle +| \Big), \\ S_z &= \frac{\hbar}{2}\sigma_z = \frac{\hbar}{2}\Big(|+\rangle\langle +| - |-\rangle\langle -| \Big). \end{aligned}$$

Along the axis parallel to a general unit vector $\hat{n}$,

$$S_n = S \cdot \hat{n}.$$

The spin up and spin down states of the operator S_n , with eigenvalues $\pm\hbar/2$, are

$$\begin{aligned} |S_n, +\rangle &= \cos\Big(\frac{\theta}{2}\Big)|+\rangle + \sin\Big(\frac{\theta}{2}\Big)e^{i\phi}|-\rangle, \\ |S_n, -\rangle &= -\sin\Big(\frac{\theta}{2}\Big)|+\rangle + \cos\Big(\frac{\theta}{2}\Big)e^{i\phi}|-\rangle. \end{aligned}$$

Inversely,

$$\begin{aligned} |+\rangle &= \cos\Big(\frac{\theta}{2}\Big)|S_n, +\rangle - \sin\Big(\frac{\theta}{2}\Big)|S_n, -\rangle, \\ |-\rangle &= \sin\Big(\frac{\theta}{2}\Big)e^{-i\phi}|S_n, +\rangle + \cos\Big(\frac{\theta}{2}\Big)e^{-i\phi}|S_n, -\rangle. \end{aligned}$$

The most general spin-$\frac{1}{2}$ state can be written as

$$|s\rangle = a|+\rangle + be^{i\delta}|-\rangle.$$

Measurement

To illustrate how to use the previous basis in a *measurement*, let us suppose that the measurement of an electron's spin along z-axis (S_z) gives $+\frac{\hbar}{2}$ and we want the probability that a subsequent measurement of the spin in the direction $\hat{n} = (\sin\theta\cos\phi, \sin\theta\cos\phi, \cos\theta)$ gives again $+\frac{\hbar}{2}$. The probability of measuring again for S_n in the state $|+\rangle$ is given by the square of the value of the overlap

$$P = |\langle S_n, +|+\rangle|^2 = \cos^2\left(\frac{\theta}{2}\right).$$

We can thinking this problem backward. Supposing the measurement of the spin along the axis $\hat{n}$ gives $+\frac{\hbar}{2}$, let us find the probability that a subsequent measurement of spin along the z-axis yields $+\frac{\hbar}{2}$,

$$P = |\langle +|S_n, +\rangle|^2 = \cos^2\left(\frac{\theta}{2}\right).$$

N spin-$\frac{1}{2}$ Particles

For N spin-$\frac{1}{2}$ particles, the total Hilbert space is

$$\mathcal{H} = \mathcal{H}_2^1 \otimes \mathcal{H}_2^2 \otimes \mathcal{H}_2^3 \otimes ... \otimes \mathcal{H}_2^N,$$

where $\mathcal{H}_2^i$ is the two-dimensional Hilbert space of the ith particle. The dimension of $\mathcal{H}$ is 2^N.

We can define the operator $S_z = S_z^i + S_z^2 + ... + S_z^N$ which acts on a product of one particle state. The eigenstates of S_z will be given by a direct product of eigenstates of each particle spin, $|+\rangle^i, |-\rangle^i$. The spectrum is given by the total number of spin up, N_+, and spin down, N_-, up to a constant, let us say $s_z = \frac{\hbar}{2}(N_+ - N_-)$, where $N_+ + N_- = N$ or

$$s_z^{N_+} = \frac{\hbar}{2}(2N_+ - N).$$

The total number of states is 2^N. The degeneracy of the state N_+ can be thought as the number of spins up of the system, i.e. the number of ways we can choose N_+ states,

$$g_{N_+} = \frac{N!}{N_+!N_-!}$$

Permutation Operator

A permutation operator is defined for any state $|\alpha\rangle, |\beta\rangle$ of two spin-$\frac{1}{2}$ particles, as the operator

$$P\Big(|\alpha\rangle \otimes |\beta\rangle\Big) = |\beta\rangle \otimes |\alpha\rangle.$$

In terms of Pauli matrices we can write the permutation operator as

$$P = \frac{1}{2}\Big(\mathbf{1} \otimes \mathbf{1} + \vec{\sigma} \otimes \vec{\sigma}\Big),$$

with eigenvalues $\lambda = \pm 1$ on the eigenstates $|\pm\rangle \otimes |\pm\rangle$.

A spin-$\frac{1}{2}$ Particle in a Magnetic Field

The Hamiltonian for the magnetic field in the x-direction is

$$H = -\mu_x \cdot B,$$

where μ_x is the spin magnetic moment

$$\mu_x = \frac{2e}{mc} S_x = \frac{\hbar e}{mc} \sigma_x.$$

1.3.3 Angular Momentum

Orbital Angular Momentum

The orbital angular momentum has the same formalism of the particle spin angular momentum, where we define the non-abelian commutation relations of the orbital angular momentum operator,

$$[L_i, L_j] = i\hbar\epsilon^{ijk} L_k.$$

It is useful to define the squared momentum operator

$$L^2 = L_z + \frac{1}{2}(L_z + L_- L_+ + L_+ L_-).$$

Example: For a state with defined by L_z, one has $\left\langle \{L_x, L_y\} \right\rangle = 0$.

Proof.

$$\{L_x, L_y\} = \frac{1}{4i}(L_+^2 - L_-^2),$$

This operator in the basis $|l, m\rangle$ has zeros on the diagonals, and therefore:

$$\langle l, m|\{L_x, L_y\}|l, m\rangle = 0.$$

□

Total Angular Momentum

The total angular momentum also obeys the same commutation rule

$$[J_i, J_j] = i\hbar\epsilon^{ijk}J_k.$$

It is useful to define the following non-hermitian raising/ lowering operators

$$J_\pm = J_x \pm iJ_y.$$

The commutation relations are

$$[J_z, J_\pm] = \pm\hbar J_\pm,$$

$$[J_+, J_-] = 2\hbar J_z.$$

Once again, we can define the squared momentum operator, which commutes to the previous operators,

$$J^2 = J_-J_+ + J_z^2 + \hbar J_z. \tag{1.3.13}$$

The eigenvalues for the total angular momentum are

$$\begin{aligned}
&J_z|j, m\rangle = \hbar m|j, m\rangle, \\
&J^2|j, m\rangle = \hbar^2 j(j+1)|j, m\rangle, \\
&J_+|j, m\rangle = \hbar\sqrt{(j-m)(j+m+1)}|j, m+1\rangle, \\
&J_-|j, m\rangle = \hbar\sqrt{(j+m)(j-m+1)}\ |j, m-1\rangle,
\end{aligned}$$

where $-j \leq m \leq j$, and one constructs $2j+1$ states. The Matrix Elements of these states are

$$\begin{aligned}
&\langle j', m'|J^2|j, m\rangle = \hbar^2 j(j+1)\delta_{mm'}\delta_{jj'},\\
&\langle j', m'|J_z|j, m\rangle = \hbar m\delta_{mm'}\delta_{jj'},\\
&\langle j', m'|J_+|j, m\rangle = \hbar\sqrt{(j-m)(j+m+1)}\delta_{mm'+1}\delta_{jj'},\\
&\langle j', m'|J_-|j, m\rangle = \hbar\sqrt{(j+m)(j-m+1)}\delta_{mm'-1}\delta_{jj'}.
\end{aligned}$$

Example: A Spin-1 System.

Let us suppose a spin-1 system given by the Hamiltonian

$$H = AS_z^2 + B(S_x^2 - S_y^2).$$

Using the spin operator $S_\pm = S_x \pm S_y$ we can write

$$H = AS_z^2 + \frac{B}{2}(S_+^2 - S_-^2).$$

From the previous formalism we can write the eigenstates

$$S_\pm|1, m\rangle = \hbar\sqrt{(1 \pm m)(1 \pm m + 1)}\ |1, m-1\rangle.$$

resulting into the following Hamiltonian,

$$H = \hbar^2 \begin{pmatrix} A & 0 & B \\ 0 & 0 & 0 \\ B & 0 & A \end{pmatrix}.$$

Spherical Harmonics

The *spherical harmonics* are eigenfunctions of the squared orbital angular momentum, (1.3.13) , and the generator of rotation about the azimuthal axis. Their general form is

$$Y_l^l(\theta, \phi) = c_l \sin^l(\theta)e^{il\phi},$$

where

$$c_l = \frac{(-1)^l}{2^l l!}\sqrt{\frac{2l+1}{4\pi}(2l)!}.$$

Example: Expectation Value of $(L_xL_y + L_yL_x)$ in the State with Angular Part of $Y_3^2(\theta, \phi)$.

Writing

$$\{L_x, L_y\} = \frac{1}{4i}\Big(L_+^2 - L_-^2\Big),$$

the expectation value in the basis $|l, m\rangle$ is

$$\langle l, m|\{L_x, L_y\}|l, m\rangle = 0.$$

Addition of Angular Momentum: Clebsch-Gordan Coefficients

Let us suppose a system of two particles, where we can define the states by four quantum numbers, let us say j_1, j_2, j, m: each angular momentum, the sum of the angular momentum and the z-component of the total angular momentum. They form a complete basis and they can be decomposed into the complete basis formed by the four quantum numbers j_1, j_2, m_1, m_2: each angular momentum and each z-component.

$$|j_1, j_2, j, m\rangle = \sum_{m_1,m_2} |j_1, j_2, m_1, m_2\rangle\langle j_1, j_2, m_1, m_2|j_1, j_2, j, m\rangle.$$

The coefficients of this change of basis (the last term scalar product of (1.3.14)) are the Clebsch-Gordan coefficients, which the following *selection rules*

- Clebsch-Gordan $= 0$ unless $m = m_1 + m_2$.
- Clebsch-Gordan $= 0$ unless $|j_i - j_2| \leq j \leq j_1 + j_2$.
- For each j_1 there are $2j_1 + 1$ values of m_1, so $N = (2j_1 + 1)(2j_2 + 1)$.
- Clebsch-Gordan coefficients form a unitary matrix.

The direct product of two spin spaces can be calculated by the rule

$$j_1 \otimes j_2 = |j_1 - j_2| \oplus |j_1 - j_2 + 1| \oplus \ ... \ \oplus j_1 + j_2,$$

where it is possible to count the sates

$$(2j + 1)(2j + 1) = \sum_{j=|j_1+j_2|}^{j_1+j_2} (2j + 1).$$

For example, for two spin-particles,

$$J = J_1 \otimes \mathbf{1} + \mathbf{1} \otimes J_2.$$

Example: Decomposing Two p-electrons.

The sum of two p-electrons can be write as

$$|l_1, l_2, l, m\rangle = |1, 1, -1, -1\rangle = \frac{1}{\sqrt{2}}(|1, 0\rangle|1, -1\rangle + |1, -1\rangle|1, 0\rangle),$$

where one has 50% probability of having $m = -1$ or $m = 0$ if measuring any of l_z.

Example: Two spin-$\frac{1}{2}$ Particles.

For one electron, one has the following the wavefunction,

$$\psi(x_1, \sigma_1) = \psi_1(x_1)|+\rangle + \psi_s(x_1)|-\rangle,$$

where the first part is from the orbital part and the second for spin. For two electrons,

$$\psi(x_1, \sigma_1, x_2, \sigma_2) = \psi_{++}|++\rangle + \psi_{+-}|+-\rangle + \psi_{-+}|-+\rangle + \psi_{--}|--\rangle.$$

The Hamiltonian commutes with the spin operator, therefore they share the same eigenkets. The sum of two spin-$\frac{1}{2}$ particles is

$$\mathbf{\frac{1}{2}} \otimes \mathbf{\frac{1}{2}} = \mathbf{0} \oplus \mathbf{1}.$$

These two resulting states are a single, $\mathbf{0}$, and triplet, $\mathbf{1}$. The triplet can be write as

$$\begin{aligned}
|1, 1\rangle &= |++\rangle = \frac{1}{2}(1, \sqrt{2}, 1), \\
|1, -1\rangle &= |--\rangle = \frac{1}{2}(1, -\sqrt{2}, 1), \\
|1, 0\rangle &= \frac{1}{\sqrt{2}}(|-+\rangle + |+-\rangle) = \frac{1}{\sqrt{2}}(1, 0, -1),
\end{aligned}$$

and the singlet,

$$|0, 0\rangle = \frac{1}{\sqrt{2}}\Big(|-+\rangle - |+-\rangle\Big) = \frac{1}{\sqrt{2}}(1, 1, 1).$$

The eigenvalues of this system are

$$\begin{aligned} L^2\psi &= \hbar^2 l(l+1)\psi, \\ S^2\psi &= \frac{3}{4}\hbar^2\psi, \\ J^2\psi &= \hbar^2 j(j+1)\psi, \\ J_z\psi &= \hbar m\psi, \\ L\cdot S\psi &= \frac{1}{2}(J^2 - L^2 - S^2)\psi \\ &= \frac{\hbar^2}{2}\Big(j(j+1) - l(l+1) - \frac{3}{2}\Big)\psi. \end{aligned}$$

Example: Decomposition of Four spin-$\frac{1}{2}$ Particles.

$$\begin{aligned} \mathbf{\frac{1}{2}}^{\otimes 4} &= (\mathbf{0}\oplus\mathbf{1})^{\otimes 2} \\ &= (0\oplus 1)\otimes\frac{1}{2}\otimes\frac{1}{2} \\ &= (\frac{1}{2}\oplus\frac{1}{2}\oplus\frac{3}{2})\otimes\frac{1}{2} \\ &= (\mathbf{0}\oplus\mathbf{0}\oplus\mathbf{1}\oplus\mathbf{1}\oplus\mathbf{2}), \end{aligned}$$

giving two singlets, two triplets and one quintuplet.

Example: Decomposition of Four p-electrons.

Four electrons in p state have $l = 1$ each for angular momentum,

$$\mathbf{1}^{\otimes 4} = (\mathbf{0}\oplus\mathbf{1}\oplus\mathbf{2})\otimes(\mathbf{0}\oplus\mathbf{1}\oplus\mathbf{2}).$$

giving $l_{tot} = 0, 1, 2, 3, 4$ values allowed.

Example: Decomposition of a System with $j_1 = \frac{1}{2}, j_2 = \frac{3}{2}, j_3 = 1$.

$$\begin{aligned} \mathbf{\frac{1}{2}}\otimes\mathbf{\frac{3}{2}}\otimes\mathbf{1} &= \mathbf{1}\otimes\mathbf{1}\oplus 2\otimes 1, \\ &= \mathbf{0}\oplus 2\cdot\mathbf{1}\oplus 2\cdot\mathbf{2}\oplus\mathbf{3}, \end{aligned}$$

which are one singlet (1 state), two triplets (6 states), two quintets (10 states) and one septet (7 states).

Tensor Operator

For higher order system, we generalize the commutation relations to

$$[J_z, T_q^k] = \hbar q T_q^k,$$

$$[J_\pm, T_q^k] = \hbar\sqrt{(k \mp q)(k \pm q + 1)}T_{q\pm1}^k,$$

resulting into the the matrix elements

$$\langle \alpha', j', m'|T_q^k|\alpha, j, m\rangle \neq 0 \text{ only if } m' = q + m.$$

The *Wigner-Eckart Theorem* is given by the relation

$$\langle \alpha', j', m'|T_q^k|\alpha, j, m\rangle = \langle j', k', m', q'|j, k, j', m\rangle.\langle \alpha'_j|T^k|\alpha_j\rangle,$$

with applications on the tensor theory such as

1. **Tensor of rank 0, scalar**: The scalar operator cannot change j, m values.

$$\langle \alpha', j', m'|S|\alpha, j, m\rangle = \delta_{jj'}\delta_{mm'}\frac{\langle \alpha'_{j'}|S|\alpha_j\rangle}{\sqrt{2j+1}}.$$

2. **Tensor of rank 1, vector**: The spherical component of the potential can be written as $V_{q=\pm1,0}$ and the selection rules are:

$$\Delta m \equiv m' - m = \pm1, 0 \;\; \Delta j \equiv j' - j = \pm1, 0. \tag{1.3.14}$$

1.3.4 Identical Particles

Let us study the *permutation symmetry* of the Hamiltonian of two particles

$$H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + V(|x_1 - x_2|) + V'(x_1) + V'(x_2).$$

If we start with a system which is permutation symmetrical, the states continue to have this propriety even if it evolutes with time. The eigenstate of the Hamiltonian and the permutation operator are

$$|k', k''\rangle = \frac{1}{\sqrt{2}}(|k'\rangle \otimes |k''\rangle \pm |k''\rangle \otimes |k'\rangle),$$

with the eigenvalues

$$P_{12}|k,k''\rangle_{\pm} = \pm|k',k''\rangle_{\pm}.$$

It is useful to define the *symmetry projectors*, one symmetrical and one anti-symmetrical projector,

$$\begin{aligned} S_{12} &= \frac{1}{2}(\mathbf{1}+P_{12}), \\ A_{12} &= \frac{1}{2}(\mathbf{1}-P_{12}), \end{aligned}$$

which commutes to the Hamiltonian,

$$P_{12}HP_{12}^{-1} = H,$$

Applying to the eigenstates,

$$\begin{aligned} S_{12}|k'\rangle \otimes |k''\rangle &= |k',k''\rangle_{+}, \\ A_{12}|k'\rangle \otimes |k''\rangle &= |k',k''\rangle_{-}. \end{aligned}$$

Many Identical Particles

We generalize the theory for many identical particles,

$$V_i \otimes Vj... \otimes V_k.$$

The permutation operator P_{ij} takes $|k_i'\rangle \otimes |k_j''\rangle$ to $|k_i''\rangle \otimes |k_j'\rangle$, with the following proprieties:

- $P_{12}^2 = 1$.
- $[P_{ij}, P_{kl}] = 0$, if $(ij)(kl) = 0$ (they do not intersect).
- $P_{12}P_{23}P_{21} = P_{23}P_{12}P_{23}$ (Braid's theory).

Fermions and Bosons

The operator permutation applied to symmetrical (bosons) or anti-symmetrical (fermions) systems gives

$$\begin{aligned} P_{ij}|fermions\rangle &= +|fermions\rangle, \\ P_{ij}|fermions\rangle &= -|fermions\rangle. \end{aligned}$$

Bosons	$\|a\rangle \otimes \|a\rangle$ $\|b\rangle \otimes \|b\rangle$ $\|a\rangle \otimes \|b\rangle + \|b\rangle \otimes \|a\rangle$	Symmetric	$P_{12}^{spin} = +1$	$P_{12}^{orb} = -1$
Fermions	$\|a\rangle \otimes \|b\rangle - \|b\rangle \otimes \|a\rangle$	Antisymmetric	$P_{12}^{spin} = -1$	$P_{12}^{orb} = +1$

Table 1.1: Spectrum for two identical Particles

Let us suppose a system of two particle, the spectrum is given by table 1.1, where one sees clearly the *principle of exclusion of Pauli*.

The permutation operator can be split as

$$\begin{aligned} P_{12}^{spin} &= \frac{1}{2}(1 + \frac{4}{\hbar^2} S_1 S_2) \\ &= \frac{1}{2}(1 - \sigma_1 \sigma_2), \end{aligned}$$

with eigenvalues $\frac{3}{4}\hbar^2$ for triplet and $\frac{1}{4}\hbar^2$ for singlet.

1.4 Density Matrix

A *density matrix* is a hermitian matrix of trace one, that describes the statistical state of a quantum system.The density matrix is useful for dealing with mixed states, i.e. statistical ensemble of two or more different systems. Before we were describing states as a coherent linear supposition, for example $|\alpha\rangle = C_+|+\rangle + C_-|-\rangle$, with only defined direction. With the density matrix formalism we can work with completely random ensembles (unpolarized), or pure ensemble (polarized), or mixed ensemble (partially polarized).

The operator that is represented by the density matrix is the density operator,

$$\rho = \sum_i w_i |\alpha^i\rangle\langle\alpha^i|. \tag{1.4.1}$$

The expected value for any operator can be calculated by

$$\langle A\rangle = \text{tr } (\rho A),$$

with

$$\text{tr } (\rho) = 1.$$

The evolution of the density operator is given by

$$i\hbar\partial_E \rho = [H, \rho].$$

The entropy is given by

$$S = -\text{tr } (\rho \ln \rho) = -\sum_i \ln\rho, \tag{1.4.2}$$

and it is additive ($S = S_1 + S_2$), which can be proved by applying the trace.

Example: Ensemble of spin-1 Systems

For spin-1 systems the density matrix is 3×3, which has $3 \cdot 3 \cdot 2 = 18$ real parameters. Since the matrix is hermitian we reduce this number to 9. Since the trace is unity, it has 8 parameters. The $[S_i]$ provide three more. Other 6 parameters come from $[S_i S_j]$, which since $[S^2] = 2\hbar^2$, gives the 5 final parameters.

1.4.1 Pure Ensemble

The pure ensemble is completely polarized. On (1.4.1), we have $w_1 = 1$,

$$\begin{aligned} \rho^2 &= \rho, \\ \text{tr}(\rho^2) &= 1, \\ S &= 0. \end{aligned}$$

Example: Finding the Reduced Density Matrix for the *first* spin-$\frac{1}{2}$ in a Pure State of *two* spin-$\frac{1}{2}$.

Let us write the two spin-$\frac{1}{2}$ given by the normalized state

$$\frac{1}{\sqrt{6}}\Big(|+\rangle \otimes |-\rangle + 2|-\rangle \otimes |+\rangle + i|+\rangle \otimes |+\rangle\Big).$$

Taking the trace with respect to the second spin gives,

$$\rho = \sum_i \langle i|\Psi\rangle\langle\Psi|i\rangle = N \begin{pmatrix} 2 & 2i \\ -2i & 4 \end{pmatrix}.$$

with the states $|i\rangle$, $i = +, -$, in the second spin space. The normalization is tr $\rho = 1$, therefore $N = \frac{1}{2}$, resulting in the reduced matrix

$$\rho = \begin{pmatrix} \frac{1}{3} & \frac{i}{3} \\ -\frac{i}{3} & \frac{2}{3} \end{pmatrix}.$$

We can decompose the density matrix as

$$\rho = \frac{1}{2}1 + \frac{1}{3}\sigma_2 - \frac{1}{6}\sigma_3,$$

which makes it easy to calculate the expectation values of the components of the operator S for the first spin in this state. The average over the spin operator is

$$\text{tr}(\rho S) = \text{ tr}(\rho S_x)\hat{x} + \text{ tr}(\rho S_y)\hat{y} + \text{ tr}(\rho S_z)\hat{z} = \frac{\hbar}{6}(2\hat{y} - \hat{z}).$$

The entropy, i.e. the entanglement, of this reduced matrix is given by the equation (1.4.2) and can be calculated by finding the eigenvalues of the density matrix. Diagonalizing ρ by $\det(\rho - \lambda 1)$, gives the eigenvalues $\lambda_\pm = \frac{1}{2} \pm \frac{\sqrt{5}}{6}$. Therefore,

$$S = -\sum_k \rho_{kk} \ln\rho_{kk} = -\sum_i \lambda_i \ln\lambda_i.$$

1.4.2 Mixed Ensemble

The random ensemble is partially polarized. The reduced matrix for an entangled pure ensemble is a mixed ensemble,

$$\text{tr } (\rho)^2 = \sum \rho_i < 1,$$
$$\frac{1}{N} \leq \text{ tr } \rho^2 \leq 1.$$

Example: Mixed Ensemble of a spin-$\frac{1}{2}$ System.

Supposing that the ensemble averages $[S_x], [S_y], [S_y]$ are known. The spin-$\frac{1}{2}$ density matrix is a hermitian 2×2 matrix with unit trace, therefore we decompose

$$\rho = \frac{1}{2} + \alpha_i \sigma^i,$$

where $\alpha_i = \frac{1}{2}$ tr $(\rho\sigma_i) = \frac{1}{\hbar}[S_i]$. Writing the spin operator as

$$[S_i] = \text{ tr}(\rho S_i) = \frac{\hbar}{2} \text{ tr}(\rho\sigma_i),$$

we find the density matrix of this ensemble,

$$\rho = \frac{1}{2}1 + \frac{1}{\hbar}[S]\sigma.$$

We have learned that the condition for an ensemble to be pure is tr $\rho^2 = 1$ and applying this condition to $[S_j]$,

$$\text{tr}(\rho^2) = \frac{1}{2} + \frac{2}{\hbar}([S_x]^2 + [S_y]^2 + [S_z]^2) = 1,$$

we can find the condition on $[S_j]$ to be a pure ensemble,

$$\sum_i [S_i]^2 = \frac{\hbar^2}{4}.$$

The same condition can be found by imposing that entropy is zero.

1.4.3 Random Ensemble

The random ensemble is completely unpolarized,

$$\begin{aligned} &\text{tr } \rho^2 = \frac{1}{N}, \\ &\frac{1}{N} \leq \rho \leq 1, \\ &S = \ \ln N. \end{aligned}$$

1.4.4 Time Evolution for Ensembles

The time evolution for ensembles is given by the Schroedinger equation,

$$i\hbar\frac{\partial}{dt} = -[\rho, H].$$

If the dynamics of an ensemble is governed by the Schroedinger equation, an ensemble which is pure at $t = 0$ cannot evolve into a mixed ensemble.

Proof. Assuming a pure quantum state $|\alpha\rangle$, the density matrix is

$$\rho = |\alpha\rangle\langle\alpha|,$$

and the time evolution

$$\dot{\rho} = \frac{1}{i}\Big(H|\alpha\rangle\langle\alpha| - |\alpha\rangle\langle\alpha H\Big) = i[\rho, H].$$

For a pure ensemble $\rho^2 = \rho$ (idempotent), giving tr $(\rho^2) = 1$, taking the derivative it on time, due the cyclic propriety of trace,

$$\frac{d}{dt}\ \mathrm{tr}\rho^2 = 2i\ \mathrm{tr}(\rho[\rho, H]) = 0,$$

therefore we conclude the condition tr $\rho^2 = 1$ is also true for all $t \neq 0$. □

1.5 Symmetries

1.5.1 Linear Transformations

In quantum mechanics, the Hamiltonian is translation invariant,

$$[H, T(a)] = 0.$$

The momentum operator is the generator of spatial translations, therefore the (continuous) translation operator is

$$T(a) = 1 - \frac{i\epsilon G}{\hbar} = e^{-\frac{i}{\hbar}a\hat{p}_z}, \tag{1.5.1}$$

The angular momentum operator is the generator of rotation of the system,

$$R(\hat{n}, \phi) = 1 - \frac{i\epsilon G}{\hbar} = e^{-\frac{i}{\hbar}\phi\hat{n}\cdot\hat{L}}.$$

1.5.2 Parity

Parity, or spacial inversion is the propriety of changing right-handed systems on left-handed (such as a mirror). In quantum mechanics we define the *parity*

operator,

$$
\begin{aligned}
&|\alpha\rangle \to \pi|\alpha\rangle, \\
&\pi^{-1}\pi = 1, \\
&\pi^2 = 1, \\
&\pi|n_\pm\rangle = \pm|n_\pm\rangle.
\end{aligned}
$$

From the commutation relation with the Hamiltonian,

$$[H, \pi] = 0,$$

we simultaneously diagonalize both operators. Therefore, $|n\rangle$, eigenstates of H, are also eigenstate of the parity operator:

$$
\begin{aligned}
\pi|n_\pm\rangle &= \frac{1 \pm \pi}{2}|n\rangle, \\
H|n_\pm\rangle &= E_n|n_\pm\rangle.
\end{aligned}
$$

The relations between parity and other relevant operators are in table 1.5.2. For the the wavefunctions, the parity operator acts as:

$$\pi|\alpha, l, m\rangle = (-1)^l|\alpha, l, m\rangle.$$

p	$\{p, \pi\} = 0$	odd	polar
x	$\{x, \pi\} = 0$	odd	polar
$S \cdot r$	$\{S \cdot r, \pi\} = 0$	odd	pseudoscalar
L	$[L, \pi] = 0$	even	axial
J	$[J, \pi] = 0$	even	axial
S	$[S, \pi] = 0$	even	axial
$L \cdot S$	$[L \cdot S, \pi] = 0$	even	scalar
$r \cdot p$	$[r \cdot p, \pi] = 0$	even	scalar

Table 1.2: Parity on operators.

Example: The Double-Well Potential.

$$\begin{aligned}
&\pi|S\rangle = |S\rangle,\\
&\pi|A\rangle = -|A\rangle,\\
&|R\rangle = \frac{1}{\sqrt{2}}(|S\rangle + |A\rangle),\\
&|L\rangle = \frac{1}{\sqrt{2}}(|S\rangle - |A\rangle),\\
&\Delta = E_a - E_s,\\
&T = \frac{2\pi\hbar}{\Delta}.
\end{aligned}$$

The time evolution is then:

$$|R\rangle \to \frac{1}{\sqrt{2}} e^{-\frac{i}{\hbar}E_s}\Big(|S\rangle \pm e^{-\frac{i}{\hbar}\Delta t}|A\rangle\Big).$$

Example: Two Operators that Anti-commute.

For two operators A and B which $\{A, B\} = 0$, we have:

$$\begin{aligned}
A(B|\Psi\rangle) &= -\alpha(B|\Phi\rangle),\\
B(A|\Psi\rangle) &= -\beta(A|\Phi\rangle).
\end{aligned}$$

Therefore the eigenvalues of A come in pairs α, $-\alpha$, and same happens for B. If one makes $A \to \pi$ and $B \to p$, it is possible to see that a state $p|\Psi\rangle$ is also a eigenstate of π.

Parity Selection Rule (Wigner)

Operators with **odd** parity have **odd** non-vanishing matrix elements only between states of **opposite** parity. Operators with **even** parity connect states with **same** parity.

$$\langle \alpha', l', m'|x|\alpha, l, m\rangle \to (-1)^{l'} \times (-1)^{l}, \tag{1.5.2}$$

$$(-1)^{l-l'+1} = 1, \tag{1.5.3}$$

$$l' - l = \text{odd}. \tag{1.5.4}$$

Analyzing for z, a spherical tensor of rank $q = 1, m = 0$, one rewrites the theorem as:

$$\langle \alpha', l', m'|z|\alpha, l, m\rangle = c^{m',m}_{j',j}\langle \alpha', j'|z|\alpha, j\rangle,$$
$$\text{The selection rules are } m = m', \Delta j = 0, \pm 1.$$

Hence $z|\alpha, j\rangle$ has opposite parity, the overlap states give non-zero contributions only for $\Delta j = \pm 1$.

1.5.3 Lattice Symmetry

The Tight Binding Hamiltonian on the 1d Lattice

$$H = -W\sum_{n=1}^{N}\left(e^{i\theta}|n\rangle\langle n+1| + e^{-i\theta}|n+1\rangle\langle n|\right).$$

Where $|n\rangle$ forms an orthonormal basis of the Hilbert space and the periodic boundary is given by $|n\rangle \equiv |n+N\rangle$. To find the spectrum of the system one uses the translational invariance. The translation operator is given by (1.5.1):

$$\begin{aligned}
&T|x\rangle = |x+a\rangle,\\
&e^{\frac{i}{\hbar}p.a}\Psi(x) = \Psi(x+a),\\
&T = \sum_n |n+1\rangle\langle n|,\\
&T^N = 1 \to T^N|t\rangle = t^N|t\rangle \to t_K = e^{\frac{2\pi i k}{n}}.
\end{aligned}$$

One then has:

$$H = -We^{i\theta}T - We^{-i\theta}T^\dagger,$$

and

$$[T, H] = 0.$$

The spectrum of the Hamiltonian is exactly the same as (1.2.6):

$$E_k = -2W\cos(\frac{2\pi k}{N} + \theta), \quad k = 0, ..., N-1.$$

1.5.4 Time Reversal

Time reversal is an anti-unitary operator:

$$\begin{aligned}
&\langle\tilde{\beta}|\tilde{\alpha}\rangle = \langle\beta|\alpha\rangle^*, \\
&\Theta(c_1|\alpha\rangle + c_2|\beta\rangle) = c_1^*\Theta|\alpha\rangle + c_2^*\Theta|\alpha\rangle, \\
&-iH\Theta = \Theta iH, \\
&\{H,\Theta\} = 0 \rightarrow H\Theta = -\Theta H.
\end{aligned}$$

Hermitian operators are odd or even under time reversal:

$$\Theta A\Theta^{-1} = \pm A.$$

It also gives a phase restriction on the matrix element of A taken with respect to time reversed state:

$$\langle\tilde{\beta}|A|\tilde{\alpha}\rangle^* = \pm\langle\beta|A|\alpha\rangle.$$

The action of the time reversal operator on other operators can be seen on table 1.3. The action of the time reversal on the the wavefunction is:

$$\begin{aligned}
&\Theta\Psi(x) = \Psi^*(x), \\
&\Theta\Psi(p) = \Psi^*(-p), \\
&\Theta|l,m\rangle = \Theta Y_l^m = (-1)^m Y_l^{-m} = (-1)^m|l,-m\rangle, \\
&\Theta^2|l,m\rangle = |l,m\rangle.
\end{aligned}$$

x	$\Theta\|x\rangle = \|x\rangle$	even
p	$\Theta\|p\rangle = \|-p\rangle$	odd
J	$\Theta J\Theta^{-1} = -J$	odd

Table 1.3: Time Reversal on operators.

If $[H,\Theta] = 0$ and E_n is not degenerate, then the wavefunction can be chosen as real. The proof is given by showing that $|n\rangle$ and $\Theta|n\rangle$ are the same state.

Example: Spin-$\frac{1}{2}$.

$$\Theta^2|\psi\rangle = -1|\psi\rangle.$$

Example: Spin Integer.

$$\Theta^2|\rangle = 1|\rangle.$$

Example: Spin J.

It acts as a rotation by 2π.

$$\Theta^2|\psi\rangle = (-1)^{2j}|\psi\rangle = \eta K e^{-\frac{i\pi J_y}{\hbar}}|\psi\rangle.$$

Where K is the complex conjugation operator, η the arbitrary phase and the exponential (1.3.12) is :

$$e^{-\frac{i\pi J_y}{\hbar}} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

An example of J integer is two electrons system or the orbital of a spinless particle. Both are given by:

$$\frac{1}{\sqrt{2}}\Big(|+-\rangle \pm |-+\rangle\Big).$$

Any system with an odd (even) number of electrons is odd(even) under Θ^2:

$$\Theta^2|l,m\rangle = (-1)^{2m}|l,-m\rangle, \text{for } m \text{ half or integer.}$$

Kramer Degeneracy

Time reversal commutes with the Hamiltonian:

$$[H,\Theta] = 0,$$

but it does not commutes to the evolution operator, i.e. it does not anticommutes to the Hamiltonian,

$$\Theta U(t,t_0) \neq U(t,t_0)\Theta.$$

It leads to a new non-trivial phase restriction.

$$\begin{aligned} e^{\frac{i}{\hbar}Ht}\Theta e^{-\frac{i}{\hbar}Ht} &= e^{\frac{2i}{\hbar}Ht}\Theta, \\ \text{so } \Theta^2|n\rangle &= |n\rangle \text{ is not possible for spin } \frac{1}{2}. \end{aligned}$$

Therefore, if the spin is $\frac{n}{2}$, the system is double degenerate, and $|n\rangle$, $\Theta|n\rangle$ must be different states. For a system composed of odd number of elements, each energy must be at least two-fold degenerated. Kramer degeneracy in a system with odd number of electrons can be lifted by an external magnetic field.

1.6 Perturbation Theory

Perturbation theory is a set of approximation methods to resolve a complicated quantum system in terms of a simpler.

1.6.1 Time-Independent for Non-Degenerated Energies

In the time-indepedent pertubation theory, for non-degenaterd energies, the Schroedinger equations for the *perturbed* and *unperturbed* systems are

$$\begin{aligned} &H|n\rangle = E_n|n\rangle, \\ &H = H_0 + \lambda V, \\ &H_0|n^0\rangle = E_n^0|n^0\rangle. \end{aligned}$$

The new states in function of the unperturbed can be expanded as

$$|n\rangle = |n^0\rangle + \lambda|n^1\rangle + \lambda^2|n^2\rangle ...,$$

with the normalization condition,

$$\langle n_0|n\rangle = 1.$$

The perturbation of the energy is given by

$$\Delta n = E_n - E_n^0 = \lambda \Delta n^1 + \lambda^2 \Delta n^2 ...$$

We then solve the Schroedinger equation,

$$(H_0 + \lambda V)|n\rangle = (E_n^0 + \Delta n)|n\rangle,$$
$$(\lambda V - \Delta n)|n\rangle = (E_n^0 - H_0)|n\rangle \text{ multiplying from the left for } \langle n^0| :$$
$$0 = \langle n^0|(\lambda V - \Delta n)|n\rangle,$$
$$|n\rangle = \frac{1}{(E_n^0 - H_0)}(\lambda V - \Delta n)|n\rangle.$$

Introducing the projection operator,

$$\phi_n = 1 - |n^0\rangle\langle n^0| = \sum_t |k^0\rangle\langle k^0|,$$

with the following proprieties,

$$\frac{1}{E_n^0 - H^0}\phi_n = \phi_n \frac{1}{En^0 - H^0} = \phi_n \frac{1}{En^0 - H^0}\phi_n,$$

allows us to write the perturbation on the states as

$$|n\rangle = |n^0\rangle + \frac{1}{(E_n^0 - H_0)}\phi_n(\lambda V - \Delta n)|n\rangle.$$

Therefore, the first order correction for the eigenstate is

$$|n^1\rangle = \frac{\phi_n}{E_n^0 - H_0}V|n^0\rangle = \sum_{m\neq n} \frac{V_{mn}}{E_n^0 - E_m^0}|n_m^0\rangle.$$

The energy correction is given by

$$\Delta n = \langle n^0|V|n\rangle, \Delta n^1 = \langle n^0|V|n^0\rangle, \Delta n^n = \langle n^0|V|n^{n-1}\rangle.$$

To find the second order of the energy correction, one needs Δn^2,

$$\Delta n^2 = \langle n^0|\frac{V\phi_n V}{E_n^0 - H_0}|n^0\rangle = \sum_{m\neq n} \frac{|V_{mn}|^2}{E_n^0 - E_m^0}.$$

Therefore, the second order correction for the eigenstate is

$$|n^2\rangle = \frac{\phi_n}{E_n^0 - H_0}V|n^1\rangle - \frac{\phi_n}{E_n^0 - H_0}\Delta n^1|n^1\rangle.$$

In the second order, *the correction to the ground state is negative.* The total energy for the Hamiltonian is then given by

$$E_n = E_n^0 + V_{nn} + \sum_k \frac{|V_{nk}|^2}{E_n^0 - E_k^0}.$$

The eigenfunction normalization is fiven by

$$Z_n = \frac{1}{\langle n|n\rangle},$$
$$Z_n = \frac{\partial E_n}{\partial E_n^0}.$$

Example: Quadratic Stark Effect.

The quadratic stark effect is the effect of a one-electron atom in an external electrical field. The Hamiltonian splits in two parts:

$$H = H_0 + V,$$
$$H_0 = \frac{p^2}{2m} + V_0(r) \text{ and } V = -e|E|z.$$

The correction on the energy is then:

$$\Delta_k = -e|E|z_{kk} + e^2|E|^2 \sum_{j\neq k} \frac{|z_{kj}|^2}{E_k^0 - E_j^0} + ...$$

With no degeneracy, $|k^o\rangle$, from selection rules, (1.5.4) $l' = l \pm 1$ and $m' = m$, is a parity state, therefore $z_{kk} = 0$. Hence, from parity/selection rules, one can see that there can be no linear Stark effect!

1.6.2 Time-Independent for Degenerated Energies

In the time-independent pertubation theory for degenerated energies, to calculate a perturbed Hamiltonian, we diagonalizes each block of this H_1,

$$H_0 = \begin{bmatrix} E_1^0 & 0 & 0 & 0 \\ 0 & E_1^0 & 0 & 0 \\ 0 & 0 & E_1^0 & 0 \\ 0 & 0 & 0 & E_2^0 \end{bmatrix}$$

$$H_1 = \begin{bmatrix} E_1^1 & X & X & X \\ X & E_1^1 & X & X \\ X & X & E_1^1 & X \\ X & X & X & E_2^1 \end{bmatrix}$$

The secondary corrections for the energies are

$|m^0\rangle$, m=1,2,3,...g,

$|l\rangle = \sum_m \langle m^0|l^0\rangle |m^0\rangle$,

$H|l^0\rangle = E_0|l^0\rangle$,

The secular equation is $\det\,(V - (E - E_0^0)) = 0$ where $\Delta l = E - E_0^0$, and the correction is $\Delta l^2 = \sum_{k\neq d} \frac{|V_{kl}|^2}{E_0^0 - E_k^0}$.

Example: The Linear Stark Effect.

Knowing that the Bohr radius is $a_0 = \frac{\hbar^2}{me^2}$, one has for the splitting of energies of the Hydrogen atom:

$$|n,l,m\rangle \to E_n = \frac{-e}{2a_0}\frac{1}{n^2}.$$

$$|1,0,0\rangle \to E = \frac{-e}{2a_0},\ \text{1s e.}$$

$$|2,0,0\rangle \to E = \frac{-e}{2a_0},\ \text{2s e.}$$

$$|2,1,\pm 1\rangle \to E = \frac{-e}{2a_0}\frac{1}{4},\ \text{2p e.}$$

$$|2,1,\pm 0\rangle \to E = \frac{-e}{2a_0}\frac{1}{4},\ \text{2p e.}$$

For the Hydrogen atom there are degeneracies for all but the ground state. The perturbation $V = -eZ|E|$ has non vanishing values only between states of opposite parity:

$$V = \begin{bmatrix} 0 & 0 & \langle 2s|V|2p, m=0\rangle & 0 \\ \langle 2p, m=0|V|2s\rangle & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

From selection rules (parity), m is the same and this matrix gives the only transition that the electron can make. Diagonalizing it,

$$\lambda = \pm\left|\left\langle 2p, m=0\middle|V\middle|2s\right\rangle\right|.$$

For example, if $n=2$, the splitting is on $2s$, $2p(m=0)$, $2p(m=-1)$ and $2p(m=1)$. The the level of energies are

- $2s+2p, (m=0)$,
- $2p, (m=\pm 1)$,
- $2s-2p, (m=0)$.

Therefore, the corrections are

$$\begin{aligned}
&\langle 2p, m=0|V|2s\rangle = 3ea_0|E|,\\
&V = 3ea_0|E|\sigma_x \text{ (on a diagonal matrix)},\\
&\Delta^1 = -3ea_0|E|,\\
&\frac{\partial\Delta}{\partial|E|} = 3ea_0.
\end{aligned}$$

The linear combination has no parity, however it is a combination that make the distance from **E** further. The state has now dipole moment.

1.6.3 Hydrogen Atom

The Hamiltonian of the hydrogen atom is given by

$$H = \frac{p^2}{2\mu} + V(r), \tag{1.6.1}$$

$$V(r) = -\frac{Ze^2}{r}, \tag{1.6.2}$$

which commutes to the angular momentum operator,

$$[H, L] = 0.$$

In spherical coordinates the Hamiltonian and the respective eigenfunctions are

$$
\begin{aligned}
H &= \frac{\hbar^2}{2m}(\frac{1}{r^2}\partial_r r^2 \partial_r - \frac{l^2}{r^2} + V(r)),\\
l^2 &= \frac{L}{\hbar} = -(\frac{1}{\sin\theta}\partial_\theta \sin\theta \partial_\theta + \frac{1}{\sin^2\theta}\partial_\phi^2),\\
\Psi_{nlm} &= R_{nl} Y_l^m(\theta,\phi).
\end{aligned}
$$

Minimizing the equation,

$$
\begin{aligned}
&\frac{\hbar^2}{2mr_o^2} - \frac{e^2}{r_0} = 0,\\
&r_o = \frac{\hbar^2}{2me^2} = a_0,\\
&E = -\frac{1}{2}\frac{me^4}{\hbar^2}.
\end{aligned}
$$

From the introduction of a new dimensionless variables ($\rho = \frac{2Z_r}{na_0}$), where $a_0 = \frac{\hbar^2}{m_e e^2}$ is the Bohr radius, it is possible to find the *Legendre* equation:

$$
\begin{aligned}
&\rho \to \infty, \sim \partial\rho^2 \longrightarrow R \sim e^{-\rho/2},\\
&\rho \to 0, \sim \rho^2 \longrightarrow \alpha(\alpha+1) = l(l+1), \text{ so } \alpha = l,\\
&\text{Resulting in: } R_{nl} = \rho^l e^{-\rho/2} f_{nl}.
\end{aligned}
$$

The solutions for $n \geq l+1$ are the Laguerre polynomials of degree n, L_{n+1}^{2l+1},:

$$
\begin{aligned}
L_n &= e^\rho \partial_\rho^n (e^{-\rho}\rho^n),\\
L_n^k &= (-1)^k \partial\rho^k L_{n+k},\\
&\int_{-\infty}^{\infty} e^{-\rho}\rho^{2l} L_{n+l}^{2l+1}(\rho)\rho^2 d\rho = \frac{2n(n+l)!^3}{(n-l-1)!}.
\end{aligned}
$$

The solutions for the radial part are:

$$
R_{nl}(r) = \left[\left(\frac{2Z}{na_0}\right)^3 \frac{(n-l-1)!}{2n(n+l)!^3}\right]^{1/2} e^{-\rho/2}\rho^l L_{n+l}^{2l+1}(\rho).
$$

The solution of the Schroedinger equation is

$$\Psi_{nlm} = R_{nl}(r)Y_l^m(\theta, \psi),$$
$$E_n = -\frac{1}{2n^2}\frac{Z^2e^2}{a_0}.$$

The degeneracy is n^2 and can be seen at figure (1.1) (without taking into account the spin, which doubles it to $2n^2$).

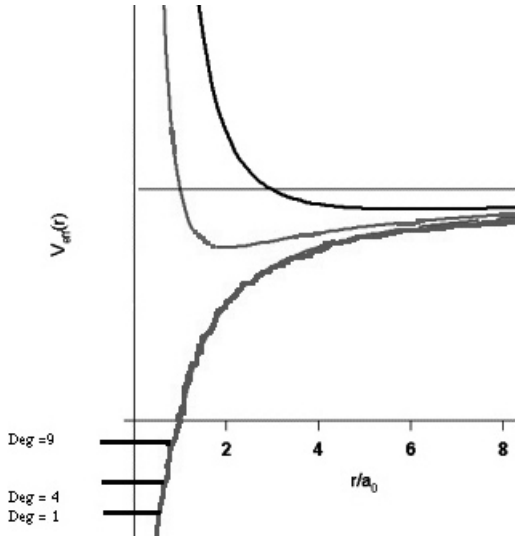


Figure 1.1: Degeneracy on the Hydrogen atom potential.

On a central potential, there is a lift of energy, which will depend on l:

$$\Delta E = \left\langle n, l, m \middle| V_o(r) - (-\frac{2e^2}{r}) \middle| n, l, m \right\rangle.$$

It is useful to have the following expected values calculated:

$$\langle r^k \rangle = \int_0^\infty \mathrm{dr}\ r^{2+k}(R_{nl}(r))^2,$$
$$\langle r \rangle = \frac{a_0}{2Z}(3n^2 - l(l+1)),$$
$$\langle r^2 \rangle = \frac{a_0 n^2}{2Z^2}(5n^2 + 1 - 3l(l+1))$$
$$\langle \frac{1}{r} \rangle = \frac{Z}{n^2 a_0} \text{ (with no splitting)},$$
$$\langle \frac{1}{r^2} \rangle = \frac{Z^2}{n^3 a_0^2 (l + \frac{1}{2})}.$$

Adding a magnetic field, the energy will also split m. The degeneracies related to the quantum numbers can be seen at table 1.4.

n	l	Name	g	g_{total}
1	0	1s	1	1
2	0	2s	1	
2	1	2p	3	4
3	0	3s	1	
3	1	3p	3	
3	2	3d	5	9

Table 1.4: Degeneracies of Hydrogen atom.

In conclusion, for the Hamiltonian of the hydrogen atom, the equation ((1.6.2)) is the gross structure, giving a energy of $E_n \sim -\frac{1}{2N^2}$. However, it is possible to include the following corrections (where $\alpha = \frac{e^2}{\hbar c} \sim \frac{1}{137}$):

- Relativistic and Spin-orbit corrections (fine structure constant) $\sim \alpha^2$;
- Radiation corrections (Lamb shift), $\sim (Z\alpha)^2 \alpha \ln \frac{1}{2}$;
- External field;
- Electro-electron interaction;
- Nuclear-spin correction (hyperfine structure), $\sim (Z\alpha)^2 \frac{m}{M}$.

Relativistic Corrections

Expanding the relativistic energy-momentum relation, one has the corrections for higher orders:

$$E = \sqrt{(mc^2)^2 + (pc)^2} = mc^2 + \frac{p^2}{2m} + \frac{p^2}{8m^2c^2}...$$

From the Dirac equation (where α, β are Dirac matrices), the Hamiltonian can be parabolically approximate to $\frac{p^2}{2m}$:

$$H_{Dir} = e\left[\alpha\left(p - \frac{e}{c}A\right) + \beta mc^2 + e\phi\right].$$

The *Foldy-Wouthuysen* transformation is:

$$H_{Dir} \approx mc^2 + \frac{1}{2m}(p - \frac{e}{c}A)^2 - \frac{p^4}{8m^3c^2} + e\phi - \frac{e\hbar}{2mc}\sigma \cdot B - \\ -\frac{e\hbar^2}{8m^2c^2}\nabla E - \frac{ie\hbar^2}{8mc^2c^2}\sigma \cdot \nabla \times E - \frac{e\hbar}{4m^2c^2}\sigma \cdot E \times p \ ...$$

The only terms that are not negligible are

$$\begin{aligned} -\frac{e\hbar}{4m^2c^2}\sigma \cdot E \times p &= -\frac{e\hbar}{4m^2c^2}\left(-\frac{1}{re}\frac{dV}{dr}\right)\sigma \cdot \frac{r \times p}{L}, \\ &= \frac{1}{2m^2e^2}\frac{1}{r}\frac{dV}{dr}L \cdot S, \end{aligned}$$

which is the correction for the spin-orbit interaction,

$$H_{LS} = \frac{1}{2m^2e^2}\frac{1}{r}\frac{dV}{dr}L \cdot S$$

Spin-Orbit Interaction and Fine Structure

Because of the central force part, the valence electron has electric field proportional to the central potential $V_c(r)$. The Hamiltonian is then:

$$H_0 = \frac{p^2}{2m} + V_c(r)$$

The perturbation for the state $|n, l, m_l, s, m_s\rangle$ is H_{LS}, where m_l and m_s are not good quantum numbers but l and s are, since $L \cdot S$ commutes to all: L^2, S^2, J^2, J_z. The degeneracy of $L \cdot S$ is $(2l-1)(2l+1)$ and this is the size of the matrix.

$$\begin{aligned}
E_{nl}^{(0)} &\rightarrow E_{nl}^{(0)} + \Delta_{nlj}, \\
\Delta_{nlj} &= \langle n, l, s, j, m| \frac{1}{2m^2c^2} \frac{1}{r} \frac{dV_c}{dr} L \cdot S |n, l, s, j, m\rangle, \\
&= \int_0^\infty \mathrm{dr}\ r^2 R_{nl}^2 \frac{1}{r} \frac{dV}{dr} \langle L \cdot S \rangle. \\
\text{But } \langle L \cdot S \rangle &= \frac{\hbar^2}{2} \bigg(j(j+1) - l(l+1) - s(s+1) \bigg), \\
\text{So, } \Delta_{nlj} &= \frac{\Delta_{nl}}{2} \bigg(j(j+1) - l(l+1) - s(s+1) \bigg).
\end{aligned}$$

For spin $s = \pm\frac{1}{2}$, there are two values for j. The Lande's interval rule gives

$$\Delta_{nlj} - \Delta_{nl(j-1)} = \Delta_{nl} \frac{1}{2} \bigg(j(j+1) - (j-1)j \bigg) = \Delta_{nlj}$$

The actual value for the splitting is then

$$\begin{aligned}
\Delta_{nlj} &\sim \langle \frac{\hbar^2}{2m^2c^2} \frac{1}{r} \frac{dV}{dr} \rangle \\
&\sim \frac{e^2}{a_o^3} \frac{\hbar^2}{m^2c^2} \\
&\sim \frac{e^2}{a_o} \frac{\hbar^2}{a_0^2 mc^2}
\end{aligned}$$

Giving the correction for fine structure,

$$\Delta_{nlj} \sim \frac{e^2}{a_0} \alpha^2,$$

order of ($\sim \frac{1}{137^2}$), and significant for f electrons.

Zeeman Effect

The Zeeman effect occurs when one applies an uniform magnetic field to the hydrogen atom,

$$\begin{aligned} B &= \nabla \times A, \\ H &= \frac{p^2}{2m} + V_c(r) - \frac{e}{2mc}(p \cdot A + A \cdot p) + \frac{e^2 A^2}{2mc^2}, \\ A &= \frac{1}{2} B \times r = -\frac{1}{2}(B_y \hat{x} - B_x \hat{y}). \end{aligned}$$

For $\nabla A = 0, p \cdot A = A \cdot p$,

$$\begin{aligned} A \cdot p &= B(-\frac{1}{2} y P_x + \frac{1}{2} x p_y) = \frac{B}{2} L_z, \\ A^2 &= \frac{1}{4} B^2 (x^2 + y^2). \end{aligned}$$

The Hamiltonian is then

$$\begin{aligned} &H \cong \frac{p^2}{2m} + V_c(r) + \frac{1}{2m_e^2 c^2} \frac{1}{r} \frac{\partial V_c}{\partial r} L \cdot S - \frac{e}{2mc} B(L_z + 2S_z), \\ &H = H_0 + H_{LS} + H_B. \end{aligned}$$

For the case which $H_B \ll H_{LS}$: H_B is treated as a small perturbation and one studies the eigenkets of $H_0 + H_{LS}$, J^2, J_z, noting that:

$$L_z + 2S_z = J_z + S_z, \text{ and } |n, l, s, j, m\rangle,$$

$$\begin{aligned} \langle L_z + 2S_z \rangle &= \langle J_z + S_z \rangle = \hbar m_j + \langle S_z \rangle, \\ |j = l \pm \frac{1}{2}, m\rangle &= \pm \sqrt{\frac{l \pm m + \frac{1}{2}}{2l+1}} |m_l \\ &= m - \frac{1}{2}, m_s = \frac{1}{2}\rangle + \sqrt{\frac{l \mp m + \frac{1}{2}}{2l+1}} |m_l \\ &= m + \frac{1}{2}, m_s = -\frac{1}{2}\rangle, \\ |j = l \pm \frac{1}{2}, m\rangle &= \pm c_+ |m_l \\ &= m - \frac{1}{2}, m_s = \frac{1}{2}\rangle + c_- |m_l \\ &= m + \frac{1}{2}, m_s = -\frac{1}{2}\rangle, . \end{aligned}$$

Therefore $\langle S_z\rangle = \frac{\hbar}{2}(|c_+|^2 - |c_-|^2) = \pm\frac{m\hbar}{2l+1}$. The correction in the energy due B is then proportional to m_j:

$$\Delta E_B = -\frac{e\hbar B}{2mc} m_j (1 \pm \frac{1}{2l+1}).$$

Now, the Lande's factor is given by

$$\langle S_z\rangle = \beta\langle J_z\rangle = \beta m_j \hbar,$$
$$g = 1 + \frac{j(j+1) + s(s+1) - l(l+1)}{2j(j+1)}.$$

For the case which $H_B \gg H_{LS}$: the term H_B is more important than H_{LS}.

$$\langle H_B\rangle = -\frac{eB\hbar}{2mc}(m_l + 2m_s),$$
$$\langle L\cdot S\rangle = \hbar^2 m_l m_s.$$

	Dominates	Good	Not Good
Weak B	H_{LS}	$J^2, L\cdot S$	L_z, S_z
Strong B	H_B	L_z, S_z	$J^2, L\cdot S$

Table 1.5: Applying a magnetic field to the hydrogen atom.

1.6.4 Time-dependent Perturbation Theory

The pertubation theory for time-dependent systems consists in finding the solutions of

$$H = H_0 + V(t),$$
$$|\alpha\rangle_t = e^{-u\frac{1}{\hbar}H_0 t}|\alpha\rangle_0,$$
$$i\hbar\partial_t|\alpha\rangle_t = H_0|\alpha\rangle_t,$$
$$i\hbar\partial_t|\alpha\rangle = (H_0 + V(t))|\alpha\rangle.$$

The Interaction Picture

The interaction in Schroedinger and Heisenberg pictures is represented by

$$\begin{aligned} |\alpha\rangle_I &= e^{\frac{i}{\hbar}E_n t}|\alpha\rangle_S \\ &= e^{\frac{i}{\hbar}H_0 t}e^{-\frac{i}{\hbar}Ht}|\alpha\rangle_H. \end{aligned}$$

Where the observables are

$$\begin{aligned} A_I &= e^{iH_0t/\hbar}A_S e^{-iH_0t/\hbar}, \\ V_I &= e^{iH_0t/\hbar}V e^{-iH_0t/\hbar}. \end{aligned}$$

The connection between the Schroedinger and Heisenberg is H instead of H_0,

$$i\hbar\frac{\partial}{\partial t}|\psi\rangle_I = i\hbar\frac{\partial}{\partial t}e^{-H_0t/\hbar}|\psi\rangle_S = e^{iH_0t/\hbar}Ve^{-iH_0t/\hbar}e^{iH_0t/\hbar}|\psi\rangle_S.$$

Therefore, the equations for the interaction picture are given by

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}|\psi\rangle_I &= V_I|\psi\rangle_I, \\ \frac{\partial A_I}{\partial t} &= \frac{1}{i\hbar}[A_I, H_0]. \end{aligned}$$

	Heisenberg	Interaction	Schroedinger
State	No Change	Evolution by V_I	Evolution by H
Observable	Evolution by H	Evolution by H_0	No Change

Table 1.6: The Interaction picture.

Dyson

The time evolution operator is the interaction picture is

$$\begin{aligned} &i\hbar\partial_t|\alpha\rangle_I = V_I|\alpha\rangle_I, \\ &|\alpha, t\rangle_I = U_I(t, t_0)|\alpha, t_0\rangle_I, \\ &i\hbar\partial_t U_I(t, t_0) = V_I(t)U_I(t, t_0), \\ &\text{Solving for the condition: } U_I(t_0, t_0) = 1. \end{aligned}$$

The transition probability can be predict with U_I, together with the time development of any stateket. If the initial state at $t = 0$ is one of the energy eigenstates of H_0, one obtains the initial stateket at later time,

$$\begin{aligned}
&U_I(,t,t_0) = 1 - \int_{t_0}^{t} V_I(t')U_I(t',t_0)dt', \\
&|i\rangle_t = U(t,t_0)|i\rangle_{t=0} = \sum_n |n\rangle\langle n|U_I(t,t_0)|i\rangle, \\
&\langle n|U_I(t,t_0)|i\rangle = e^{\frac{i}{\hbar}(E_n t - E_i t_0)}\langle n|U(t,t_0)|i\rangle.
\end{aligned}$$

The term $\langle n|U(t,t_0)|i\rangle$ is the transition amplitude ($\approx C_n^{(0)} + C_n^{(1)} + C_n^{(2)}$ ...). The probability of transition $i \to n$ is

$$P(i \to n) = |C_n^{(1)}(t) + C_n^{(2)}(t)...|^2.$$

Constant Perturbation

In a system with a given constant pertubation, we can represent the problem as

$$\begin{aligned}
&V(t) = V\theta(t), \\
&H = H_0 \text{ for } t < 0, \\
&H = H_0 + V(t) \text{ for } t > 0, \\
&(H_0 + V)|\tilde{n}\rangle = \tilde{E}_n|\tilde{n}\rangle, \\
&|i\rangle = \sum_{\tilde{n}} |\tilde{n}\rangle\langle\tilde{n}|i\rangle, \\
&|i\rangle_t = \sum_{\tilde{n}} e^{-\frac{i}{\hbar}\tilde{E}_n t}|\tilde{n}\rangle\langle\tilde{n}|i\rangle.
\end{aligned}$$

This is not exactly the previous results from the perturbation series, here

we should calculate the following coeficients,

$$\begin{aligned} C_n^{(0)} &= \delta_{in}, \\ C_n^{(1)} &= -\frac{i}{\hbar}\int_0^t d\tau e^{i\omega_{ni}\tau}V_{ni}(\tau)d\tau, \\ &= \frac{V_{ni}}{E_n - E_i}(1 - e^{i\omega_{ni}\tau}). \\ |C_n^{(1)}|^2 &= \frac{4|V_{ni}|^2}{E_n - E_i}(2 - 2\cos\omega_{ni}t), \\ &= \frac{4|V_{ni}|^2}{E_n - E_i}\,\sin^2(\frac{E_n - E_i}{2\hbar}t), \end{aligned}$$

In particular, when $E_n \sim E_1$,

$$\begin{aligned} |C_n^{(1)}|^2 &= \frac{|V_{ni}|^2}{\hbar^2}\frac{\sin\frac{\omega_{ni}t}{2}}{(\frac{\omega_{ni}}{2})^2}, \\ &= \frac{|V_{ni}|^2}{\hbar^2}t^2 \text{ for } t \ll \frac{\hbar}{|V_{ni}|}. \end{aligned}$$

Defining $\omega = \frac{E_n - E_i}{\hbar}$, when t becomes large, $|C_n^{(0)}|^2$ is appreciable only for those final states that satisfies,

$$t \sim \frac{2\pi}{|\omega|} = \frac{2\pi\hbar}{|E_n - E_i|}.$$

For states with exact energy conservation ($E_n = E_i$), the transition amplitude is quadratic in t,

$$|C_n(t)|^2 = \frac{1}{\hbar^2}|V_{ni}|^2t^2.$$

A transition with appreciable probability is possible in the range of the Uncertainty Principle,

$$\Delta t \cdot \Delta E \sim \hbar.$$

When the interaction time is finite, the energy conservation is not perfect and the spread of ΔE of values of $E_f - E_i$ is $T\Delta E > c\hbar$. The total probability

of particle goes to state:

$$\sum_n |C_n^{(1)}|^2 = \int_{E\sim E_1} dE\rho(E)|C_n^{(1)}|^2,$$
$$= \int dE_n \rho(E_n) Y \sin^2(\frac{E_n - E_1}{2\hbar}t)\frac{|V_{ni}|^2}{|E_n - E_i|^2},$$

with

$$\mathrm{Lim}_{\alpha\to\infty}\frac{1}{\pi}\frac{\sin^2(\alpha x)}{\alpha x^2} = \delta(x),$$
$$\int_{-\infty}^{\infty}\frac{\sin^2\omega t}{\omega^2}d\omega = \pi T,$$

resulting in

$$\sum_n |C_n^{(1)}|^2 = |V_{ni}|^2\frac{\pi t}{2\hbar}\delta(E_n - E_i)$$

The transition rate from a state i to a state n (transition per unit of time) is giving by the Fermi golden rule, which is a law of conservation of energy,

$$\frac{d\rho}{dt} = \frac{d}{dt}\sum_n |c_n^{(1)}|,$$
$$W_{i\to n} = \frac{2\pi}{\hbar}|\bar{V}_{ni}|^2\rho(E_n),$$
$$W_{i\to n} = \frac{2\pi}{\hbar}|V_{ni}|^2\delta(E_n - E_i).$$

The second order of this pertubation theory is giving by

$$\begin{aligned} C_n^{(2)} &= (-\frac{i}{\hbar})^2\sum_m V_{nm}V_{mi}\int_0^t dt' e^{i\omega_{nm}t'}\int_0^{t'} dt'' e^{i\omega_{ni}t''}, \\ &= \frac{i}{\hbar}\sum_m \frac{V_{nm}V_{mi}}{E_n - E_i} i n t_0^t (e^{-i\omega_{ni}t'} - e^{i\omega_{nm}t'})dt'. \end{aligned}$$

The transition from a state i to a state n for the second order can be seen as virtual transitions between the states, where the energy not need to be conserved.

$$W_{i\to n} = \frac{2\pi}{\hbar}|V_{ni} + \sum_m \frac{V_{nm}V_{mi}}{E_i - E_m}|^2\rho(E_n)\Big|_{E_n=E_i}.$$

Harmonic Perturbations

In harmonic perturbations, the appreciate transitions occurs only if $E_n \sim E_i$. For a harmonic oscillator, $\omega_n \to \omega_{ni} \pm \omega$. A example is an atom exposed to an uniform time dependent electric field, giving the perturbation $E(t)d$. Problems of this kind gives perturbation of the form $V(t) = p(t)Q$, where $p(t)$ is a numerical function and Q is an observable.

$$V(t) = V_0 e^{i\omega t} + V_0^\dagger e^{-i\omega t}, \text{ for } t > 0.$$
$$0, \text{ for } t < 0.$$

For first order of the pertubation theory, one has

$$\begin{aligned} C_n^{(1)} &= -\frac{i}{\hbar}\int_0^t V_{ni}(t')e^{i\omega_{ni}t'}dt', \\ &= \frac{1}{\hbar}\left(\frac{1-e^{i(\omega+\omega_{ni})t}}{\omega+\omega_{ni}}V_{0ni} + \frac{1-e^{i(\omega_{ni}-\omega)t}}{-\omega+\omega_{ni}}V_{0ni}^\dagger\right), \end{aligned}$$

which are applicable only if $E_k^0 - E_n^0 \neq \pm\hbar\omega$ or $\omega_{ni} = \frac{E_n - E_i}{\hbar} \neq \omega$. For the limits $t \to \infty$, one has the two possibilities. Hence, $|C_n^1|^2$ is appreciable for

- **Stimulated Emission**: $\omega_{ni} + \omega \sim 0$, or $E_n \sim E_1 - \hbar\omega$.
- **Absorption**: $\omega_{ni} - \omega \sim 0$, or $E_n \sim E_1 + \hbar\omega$.

$$W_{i\to n} = \frac{2\pi}{\hbar}\widehat{|V_{0ni}|}^2\rho(E_n),$$
$$W_{i\to n} = |V_{0ni}^\dagger|^2.$$

For a single level (since $V_{0ni}^\dagger = V_{0in}$),

$$W_{i\to n} = \frac{2\pi}{\hbar}(|V_{0ni}|^2)\delta(E_n - E_i \pm \hbar\omega).$$

Resulting that the probabilities of transition are the same,

$$\frac{W_{i\to n}}{\rho(E_n)} = \frac{W_{n\to i}}{\rho(E_i)}$$

The time perturbation can be regarded as a source of energy. For continuous generalization, we have $E_{min}^0 - E_n^\nu$, where E_{min} is the lowest of the continuous states. The probability of transition per unit of time is:

$$d\omega_{fi} = \frac{2\pi}{\hbar}|F_{fi}|^2\delta(E_f - E_i^0 - \hbar\omega)d\nu.$$

1.7 Other Techniques

1.7.1 The WKB Approximation

From the Schroedinger equation, one can input a solution of the kind

$$\psi = e^{\frac{i}{\hbar}\sigma}, \tag{1.7.1}$$

resulting in (when$\hbar \to 0$) ,

$$\frac{1}{2m}(\nabla\sigma)^2 = E - U.$$

Expanding σ as

$$\sigma = \sigma_0 + \hbar\sigma_1 + \hbar^2\sigma_2...$$

the zeroth order will be

$$(\hbar^0) \to \frac{1}{2m}\sigma_1^2 = E - U,$$
$$\sigma_0 = \pm\int^x \sqrt{2m(E - U(x))}dx = \pm\int^x p(x)dx.$$

Equation (1.7.1) has the classical *action* in its exponential. For the conditions $\hbar\sigma_0' \ll \sigma_0^2$ or $\vec{p}' \ll p^2$ or $k' \ll k^2$, it is trure that $\frac{1}{k} = \frac{\lambda}{2\pi} \ll 1$, and one has

$$\frac{dp}{dx} = \frac{d}{dx}\sqrt{2m(E-U)} = -\frac{m}{p}\frac{U}{dx} = \frac{mF}{p},$$
$$F = \frac{pp'}{m} \text{ where } p' = \frac{mF}{p},$$
$$\frac{\hbar\partial p}{\partial x} \ll p^2\frac{\hbar mF}{p^3} \ll 1, \frac{\partial k}{\partial x} \ll k^2.$$

thus, for $p = 0$, we have the violation of the classical turning points.The first order of this expansion is

$$(\hbar^1) \to \sigma_0'\sigma_1' + \frac{1}{2}\sigma_0'' = 0,$$
$$\sigma_1' = -\frac{1}{2}\frac{\sigma_0''}{\sigma_0'} = -\frac{1}{2}\frac{p'}{p},$$
$$\sigma_1 = -\frac{1}{2}\ln p.$$

The wavefunction is given by

$$\psi = \frac{c_1}{\sqrt{\chi}} e^{-\frac{i}{\hbar}\int^x \chi(x)dx} + \frac{c_2}{\sqrt{\chi}} e^{-\frac{i}{\hbar}\int^x \chi(x)dx}.$$

The second order will be

$$\begin{aligned}
&(\hbar^2) \to \sigma_0'\sigma_2' + \frac{1}{2}\sigma_2'^2 + \frac{1}{2}\sigma_1'' = 0, \\
&\sigma_2 = \frac{1}{4}\frac{mF}{p^3} + \frac{1}{8}m^2 \int \frac{F^2}{p^5}dx, \\
&\psi = \frac{const}{\sqrt{p}}\Big(1 - \frac{1}{4}im\hbar\frac{F}{p^3} - \frac{1}{8}i\hbar m^2 \int \frac{F^2}{p^5}dx\Big) e^{\frac{i}{\hbar}\int pxdx}.
\end{aligned}$$

Connection Formulas

One can use the classical approximation for the turning points to connect the solutions. The connection formulas, for a and b, are the turning points in $E = V(a) = V(b)$, for $x \gg 0$,

$$\begin{aligned}
a \to \psi(x) &= \frac{A}{\sqrt{\chi(x)}} e^{-\int_a^x \chi(x)dx} + \frac{B}{\sqrt{\chi(x)}} e^{\int_a^x \chi(x)dx}, \\
b \to \psi(x) &= \frac{C}{\sqrt{\chi(x)}} e^{-\int_a^x k(x)dx} + \frac{D}{\sqrt{\chi(x)}} e^{\int_a^x k(x)dx}.
\end{aligned}$$

For $x \sim a$,

$$\begin{aligned}
&V(x) - E \sim g(x-a), \\
&\frac{-\hbar}{2m}\psi'' + g(x-a)\psi = 0, \\
&z = (\frac{2mg}{\hbar^2})^{\frac{1}{3}}(x-a).
\end{aligned}$$

The solutions are $\psi = A_i(z)$ and $\psi = B_i(z)$. Using the limit $|\hbar\frac{dp}{dx} \ll p^2|$,

one has $|z| \ll \frac{1}{2}$,

$$
\begin{aligned}
A_i(z) &= \frac{1}{2\sqrt{\pi}} z^{-\frac{1}{4}} e^{-\xi}, \\
B_i(z) &= \frac{1}{2\sqrt{\pi}} z^{-\frac{1}{4}} e^{\xi}, \\
&\text{where } \xi = \frac{2}{3}|z|^{\frac{3}{2}}, \\
A_i(z) &\sim \frac{1}{\sqrt{\pi}} \cos(\xi - \frac{\pi}{4}), \\
B_i(z) &\sim -\frac{1}{\sqrt{\pi}} \sin(\xi - \frac{\pi}{4}).
\end{aligned}
$$

For $z < 0$,

$$
\begin{aligned}
\int_x^{a'} k(x)dx &= \int_x^a \sqrt{2m(E - V(\alpha)}dx, \\
&= \frac{2}{3}(\frac{2mg}{\hbar^2})^{\frac{1}{2}}(a-x)^{\frac{3}{2}}, \\
&= \xi.
\end{aligned}
$$

Hence, when $x \to \infty$,

$$
\frac{2A}{\sqrt{k(x)}} \cos(\int_x^a k(x)dx - \frac{\pi}{4}) - \frac{B}{\sqrt{k(x)}} \sin(\int_x^a k(x)dx - \frac{\pi}{4}) =
$$
$$
\frac{A}{\sqrt{\chi(x)}} e^{-\int_x^a \chi(x)dx} - \frac{B}{\sqrt{\chi(x)}} e^{\int_x^a \chi(x)dx}.
$$

Repeating the same procedure for $x - a \to b - x$ (reflected solutions) we have the whole solution.

Bound States

For bound stater, there are two additional conditions,

$$
\begin{aligned}
\psi &= \frac{1}{\sqrt{\chi(x)}} e^{\int_x^b \chi(x)dx}, \\
\psi &= \frac{2}{\sqrt{k(x)}} cos(\int_a^x k(x)dx - \frac{\pi}{4}).
\end{aligned}
$$

Making zero the wrong increasing/decreasing parts, we normalize them and we have the bound states. Requiring the cosine part to be zero and

$$\int_b^a k(x)dx = \pi(n + \frac{1}{2}.$$

We then minimize this, in such way that the phase space results in

$$2\int_b^a pdx = (n + \frac{1}{2})\hbar\pi.$$

Example: Triangular Potential Well.

The problem of the triangular potential well is given by

$$\begin{aligned} &V(x) = g(x), \\ &\frac{-\hbar^2}{2m}\psi'' + g|x|\psi = E\psi, \\ &z = (\frac{2mg}{\hbar^2})^{\frac{1}{3}}(x - \frac{F}{g}). \end{aligned}$$

The wavefunction is

$$\begin{aligned} \psi &= A_1(z), \\ \psi_n(x) &= A_1[(\frac{2mg}{\hbar^2})^{\frac{1}{3}}(x - \frac{F}{g})], \\ &= A_i'[-(\frac{2mg}{\hbar^2})^{\frac{1}{3}}\frac{E_n}{g}], \\ &= 0. \end{aligned}$$

The eigenenergies are

$$2\int_0^{\frac{E}{g}} \sqrt{\frac{2m}{\hbar}(E - gx)dx} = (n + \frac{1}{2})\pi.$$

Example: Instanton in a Double Potential Well.

Let us consider the example of an instanton in a double well potential, which solutions are

$$\psi_\pm = \frac{1}{\sqrt{2}}[\psi_0(x) \pm \psi_0(-x)],$$
$$\psi_0'' + \frac{2m}{\hbar^2}(E_0 - V(x))\psi_0 = 0,$$
$$\psi_\pm'' + \frac{2m}{\hbar}(E_\pm - V(x))\psi_\pm = 0$$

Multiplying them and integrating over the infinite yields

$$\int_0^\infty (\psi_0''\psi_\pm - \psi_\pm''\psi_0) + \frac{2m}{\hbar^2}(E_0 - E_\pm)\int_0^\infty dx\psi_0\psi_\pm = 0,$$
$$\psi_\pm(x) = \frac{1}{\sqrt{2}}(\psi_0(x) \pm \psi_0(-x)),$$
$$\psi_\pm'(x) = \frac{1}{\sqrt{2}}(\psi_0'(x) \pm \psi_0'(-x)),$$

results in

$$-\sqrt{2}\psi_0'\psi_0 + \frac{2m}{\hbar^2}(E_0 - E_{\pm\atop\mp})\frac{1}{\sqrt{2}} = 0,$$
$$E_\pm - E_0 = \mp\frac{\hbar^2}{m}\psi_0'\psi_0|_{x=0}.$$

We calculate $\psi_0'\psi_0$ using the WKB method

$$\psi_0(x) = \frac{A}{\sqrt{k(x)}}\cos(\int_a^x k(x)dx - \frac{\pi}{4}),$$
$$1 = \int_a^b \psi_0^2(x)dx = A^2\frac{\hbar\tau}{4m},$$

where one can express it the classical oscillation frequency $\omega = \frac{2\pi}{\tau}$. The

wavefunction and eigenenergies is then given by

$$\begin{aligned}
\psi_0(x) &= \sqrt{\frac{2m\omega}{\pi\hbar}}\cos\frac{1}{\sqrt{k(x)}}(\int_a^x k(x)dx - \frac{\pi}{4}),\\
&= \frac{A}{2\sqrt{\chi(x)}}e^{\int_a^x \chi(x)dx},\\
&= \frac{A}{2\sqrt{\chi(x)}}\chi(x)e^{\int_a^x \chi(x)dx},\\
\psi_0\psi_0'\Big|_{x=0} &= \frac{A^2}{4}e^{-2\int_0^a \chi(x)dx},\\
&= \frac{m\omega}{2\pi\hbar}e^{-2\int_0^a \chi(x)dx},\\
E_\pm - E_0 &= \mp\frac{\hbar\omega}{2\pi}e^{-2\int_0^a \chi(x)dx}.
\end{aligned}$$

The symmetrical splitting for $x \gg 0$, is

$$\Delta E = \frac{\hbar\omega}{\pi}e^{\int_{-a}^{a}},$$

where $\frac{\hbar\omega}{\pi} \sim 2\pi f$ is the transmission amplitude, the frequency of trying to penetrate: the particle can penetrate and then it splits the energy.

Transmission through the Barrier

The problem of the transmission through a barrier can be solved by dividing it in three distint solutions for each region and then perfoming the connection of these three parts,

$$\begin{aligned}
\psi_1(x) &= \frac{A}{\sqrt{k(x)}}e^{-\int_a^x k(x)dx} + \frac{B}{\sqrt{k(x)}}e^{-\int_a^x k(x)dx}, (x \ll a),\\
\psi_2(x) &= \frac{C}{\sqrt{\chi(x)}}e^{\int_a^x \chi(x)dx} + \frac{D}{\sqrt{\chi(x)}}e^{\int_a^x \chi(x)dx}, (a \ll x \ll b),\\
\psi_3(x) &= \frac{F}{\sqrt{k(x)}}e^{i\int_a^x k(x)dx} + \frac{G}{\sqrt{k(x)}}e^{-\int_a^x k(x)dx}, (x \gg b),
\end{aligned}$$

$$\begin{pmatrix} A \\ B \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 2\theta + \frac{1}{2\theta} & i(2\theta - \frac{1}{2\theta}) \\ -i(2\theta - \frac{1}{2\theta}) & 2\theta + \frac{1}{2\theta} \end{pmatrix}\begin{pmatrix} G \\ F \end{pmatrix},$$

where

$$\theta = e^{\int_a^b \chi(x)dx}.$$

The transmission coefficient is

$$T = \frac{|\psi_{trans}|^2 v_{trans}}{|\psi_{inc}|^2 v_{inc}} = \left|\frac{\psi_T\sqrt{K_T}}{\psi_I\sqrt{k_I}}\right| = \left|\frac{F}{A}\right|^2.$$

If $G = 0$,

$$A = M_{11}F = \frac{1}{2}(2\theta + \frac{1}{2\theta})F,$$
$$T = \frac{1}{|M_{11}|^2} = \frac{4}{(2\theta + \frac{1}{2\theta})^2} \sim \frac{1}{\theta^2} = e^{-2\int_b^a \chi(x)dx}.$$

Example: Nuclear Fusion.

Classically only high energies allow nuclear fusion, however, in quantum mechanics, there is always a possibility of penetration. The potential and energies of this problem is

$$V = \frac{Z_1 Z_2 e^2}{x},$$
$$E = \frac{Z_1 Z_2 e^2}{a},$$

To solve it, we just integrate it from a to b,

$$\begin{aligned}\int_a^0 \chi(x)dx &= \sqrt{\frac{2mE}{\hbar^2}}\int_a^0 \sqrt{\frac{a}{x} - 1}dx, \\ &= \frac{Z_1 Z_2 e^2 \pi}{\hbar V}.\end{aligned}$$

The transmission coefficient is the dominant term which defines the probability of nuclear fusion,

$$\begin{aligned}T &= \frac{1}{\theta^2}, \\ &= e^{-2\pi Z_1 Z_2 alpha \frac{c}{V}},\end{aligned}$$

which means that increasing the size of the nucleus, we have a reduction the probability of transmission.

Reflection by a Barrier

Classically we should have no turning point for a barrier with potential energy bigger thant the energy of the particle,

$$\psi \sim \frac{1}{\sqrt{k(x)}} e^{-\int_0^x k(x)dx},$$
$$V(x) = -\frac{1}{2}ax^2.$$

However, in quantum mechanics we find one turning point,

$$x_0 = \pm i\sqrt{\frac{2E}{a}},$$

which solving gives a reflection coefficient

$$\begin{aligned} R &= |r|^2, \\ &= e^{-4}\frac{\pi}{4\pi}\sqrt{ma}\frac{2E}{a}, \\ &= e^{-2\pi\epsilon}, \end{aligned}$$

where $\epsilon = \frac{E}{\hbar}\sqrt{\frac{m}{a}}$.

1.7.2 The Adiabatic Approximation

An adiabatic approximation is valid in a system which gradually changes conditions, allowing it to adapt its configuration, hence the probability density is modified by the process. If the system starts in an eigenstate of the initial Hamiltonian, it will end in the corresponding eigenstate of the final Hamiltonian.

$$H(t)\Psi = i\hbar\partial_t\Psi.$$

You can solve it instantaneous, with asymptotically good solutions

$$
\begin{aligned}
&H(t)\Psi_n(t) = E_n(t)\Psi_n(t),\\
&\Psi_n = \Psi_n e^{-\frac{i}{\hbar}E_n t},\\
&\Psi(t) = \sum_n c_n(t)\Psi_n(t)e^{i\theta_n(t)},\\
&\theta_n = -\frac{1}{\hbar}\int_0^t E(t')dt',\\
&\sum_n \dot{c}_n\psi_n e^{i\theta_n} = -\sum_n c_n\dot{\psi}_n e^{i\theta_n},\\
&\sum_n \dot{c}_n\delta_{nm} e^{i\theta_n} = -\sum_n c_n\langle\Psi_m|\dot{\Psi}_m\rangle e^{i\theta_m},\\
&\dot{c}_m = -\sum_n c_n\langle\Psi_m|\dot{\Psi}_m\rangle e^{i(\theta_n-\theta_m)},
\end{aligned}
$$

resulting in

$$\dot{H}\Psi_n + H\dot{\Psi}_n = \dot{E}_n\psi_m + E_n\dot{\Psi}.$$

So far, all the previous results were exacts. Now we multiply then by $\langle\Psi_m|$, giving

$$\langle\Psi_m|\dot{H}|\Psi_n\rangle + E_m\langle|H|\dot{\Psi}_n\rangle = \dot{E}_n\delta_{nm} + E_n\langle\Psi_m|\dot{\Psi}_n\rangle.$$

Supposing $m \neq n$, we get

$$
\begin{aligned}
c_m(t) &= c_m(0)e^{i\gamma_m(t)},\\
\gamma_m(t) &= i\int_0^t \langle\Psi_m(t')|\frac{\partial}{\partial t'}\Psi_m(t')\rangle dt',
\end{aligned}
$$

where the last is the *Berry's phase* (geometrical). The phase of the adiabatic approximation is constituted of a geometrical and a dynamics part. The final solution is then

$$\Psi = \sum_n \Psi_n(t)e^{i\theta_n(t)}e^{i\gamma_n(t)}c_n(0).$$

Example: Spin-$\frac{1}{2}$ particle in a $\vec{B}$ changing slowing with t.

Let us consider a system of a spin-$\frac{1}{2}$ particle in a magnetic field which is changing slowing with time,

$$\begin{aligned} &i\hbar\partial_t\Psi = -\mu B(t)\sigma\Psi, \\ &B(t) = B(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta). \end{aligned}$$

In an adiabatic problem, first one has to solve the instantaneous time-independent Hamiltonian and then diagonalize the equation. The eigenvalues in this case will be: $\mp\mu B(t) = E_\pm(t)$. The phase results to be

$$\theta_\pm(t) = -\frac{1}{\hbar}\int_0^t dt'\ \mathrm{Im}B(t').$$

Diagonalizing it again gives the ground states for this metric,

$$\chi_+ = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2}e^{i\phi} \end{pmatrix}, \chi_- = \begin{pmatrix} \sin\frac{\theta}{2}e^{-i\phi} \\ -\cos\frac{\theta}{2} \end{pmatrix}.$$

Now, calculating the Berry's phase in the system in the ground system, results in

$$\begin{aligned} \gamma_-(t) = \int_0^t dt'(\sin\frac{\theta}{2}e^{i\phi}, -\cos\frac{\theta}{2})i\partial_t \begin{pmatrix} \sin\frac{\theta}{2}e^{-i\phi} \\ -\cos\frac{\theta}{2} \end{pmatrix}, \\ = \int_0^t dt' \sin^2\frac{\theta}{2}\dot{\phi}, \\ = \frac{\Omega}{2}, \end{aligned}$$

which is the solid angle, and this term correspond to a piece of area (clearly a geometrical phase).

1.7.3 Scattering Theory

The amplitude of scattering is can be writen as

$$\begin{aligned} f(k',k) &= -\frac{1}{4\pi}\frac{2m}{\hbar^2}(2\pi)^3\int\frac{e^{ik'x'}}{(2\pi)^{\frac{3}{2}}}V(x')\langle x'|\psi^\dagger\rangle, \\ &= -\frac{1}{4\pi}(2\pi)^3\frac{2m}{\hbar^2}\langle k'|V|\psi^\dagger\rangle. \end{aligned}$$

The differential cross section is given by the number of scattered particles into $d\Omega$ per time over the number of incident particles crossing per time.

$$\frac{d\sigma}{d\Omega}d\theta = \frac{r^2|j_{scat}|}{|j_{inc}|} = |f(k',k)|^2 d\omega$$

The Born Approximation

If the effect of the scatterer is not too strong we can make

$$\langle x'|\psi^\dagger\rangle \to \langle x'|\phi\rangle = \frac{e^{ikx'}}{(2\pi)^{\frac{3}{2}}}$$

The approximation for the amplitude is then

$$f(k',k) \;\; = \;\; -\frac{2m}{\hbar^2}\frac{1}{q}\int_0^\infty rV(r)\sin qr dr.$$

The condition of applicability is given when $\langle x|\psi^\dagger\rangle$ is not very different from $\langle x|\phi\rangle$. At the center of the scattering, $x \sim 0$, is

$$|\frac{2m}{\hbar^2}\frac{1}{4\pi}\int d^3x' \frac{e^{ikr'}}{r'}V(r')e^{ikx'}| \ll 1.$$

Chapter 2

Anyons

```
"Composites formed from charged particles and vortices in
 (2+1)-dimensional models or fluxes tubes in 3-dimensional
     models, can have any (fractional) angular momentum.
   The statistics of these objects (spins) interpolates
  continuously between the usual boson and fermion cases."
   (Frank Wilczek, 1982, when we invented the name anyon)
```

Anyons are quasiparticles in a two-dimensional space. Anyons and charge fractionalization typically occur in strongly correlated electron systems with broken time reversal symmetry. Strong correlated means that many-body wavefunctions Ψ cannot be written as a single *Slater* determinant of the constituent electron single-particle states.

The world lines of two anyons cannot cross or merge. This allows braids to be made that make up a particular circuit. In the real world, anyons form from the excitations in an electron gas in a very strong magnetic field, and carry fractional units of magnetic flux in a particle-like manner. This phenomenon is called the *fractional quantum Hall effect*.

In 2005, [GCZ05], Vladimir Goldman, Fernando E. Camino, and Wei Zhou were said to have created the first experimental evidence for using fractional quantum Hall effect to create actual anyons, although others have suggested their results could be the product of phenomena not involving anyons. It should also be noted that nonabelian anyons, a species required for topological quantum computers, have yet to be experimentally confirmed.

The original proposal for topological quantum computation is due to Alexei Kitaev in 1997, [KIT97].

2.1 Aharonov-Bohm effect

2.2 Fractional Quantum Hall effect

2.3 First Detection of Anyons at Stony Brook

Chapter 3

Quantum Mechanics of an Open System

Part II

Fundamentals of Computer Science

Chapter 4

Introduction to Classical Computation

Quantum complexity theory has emerged alongside
the first efficient quantum algorithms in an attempt to
formalize the notion of an efficient algorithm. In analogy
to classical complexity theory, several new quantum
complexity classes have appeared. A major challenge
today consists in understanding their structure and the
interrelation between classical and quantum classes.
(Kempe, Kitaev, and Regev, 2008)

4.1 Turing Machines

The modern computer science starts with Alan Turing's paper, in 1936, [TUR36], where he developed the notion of we call a programmable computer. He showed that there is a *Universal Turing Machine* that can be used to simulate any other Turing machine. The *Church-Turing thesis* is given by

Any algorithm process can be simulated efficiently
using a probabilist Turing Machine.

The growing power of computer hardware was predicted by Gordon Moore, 1965, [MO65], known as the *Moore's Law*, stating that computer power will double for constant cost once every two years. This law have been correct,

but it should stop in the next years, due the difficulty of size and to quantum effects that begin to interfere in the functioning of the electric devices.

This is when quantum computation begins. While an ordinary computer can be used to simulate a quantum computer, it appear to be impossible to perform the simulation in an *efficient way*, therefore, quantum computers offer a speed advantage over classical computers.

The term *efficient* or *inefficient* for algorithms is precisely defined by the *computational complexity theory*. An efficient algorithm runs in *polynomial time* to the size of the problem. An inefficient algorithm runs in *superpolynomial* (e.g. exponential) time.

4.2 Classical Circuits

Any classical circuit can be replaced by an equivalent circuit with only reversible elements, by using the *Toffoli gate*. Two of the bits are control bits and one is the target bit, fliped if both control bits are 1. Applying the Toffoli gate twice make the state to return to its inital state,

$$(a, b, c) \rightarrow (a, b, c \oplus ab) \rightarrow (a, b, c).$$

4.3 Complexity Classes

4.3.1 P

4.3.2 NP

Eventually we hear about the claimed proof of $PN = P$ or $PN \neq P$. This problem, however, is still open. A interesting list of claimed proofs was resumed on [WO11] and a compendium of NP optimization problems,[CK05], collects approximability results of the NP-hard optimization, since no NP-complete problem can be solved in polynomial time (unless $P = NP$).

4.3.3 PSPACE

PSPACE contains NP and P and is defined for those problems that a classical computer can solve only using a polynomial amount of memory but requires an exponential number of steps. An example of problems are the $n \times n$ Chess or Go.

4.3.4 BQP

BQP (functions computable with bounded error,given quantum resources, in polynomial time), defines how the class of problems that quantum computers would solve efficient. This class includes all the P problems and also a few other NP problems (e.g. factoring and and discrete logarithm problem). However other NP and all NP-complete problems are believed to be outside BQP, which means that even our quantum computer may require more than a polynomial number of step to solve the problems.

BQP is also believed to be bigger than NP, which means that quantum computers may solve some problems faster than classical computers can check the answers.

4.4 Complexity of Arithmetic Operations

4.5 Probabilistic Algorithms

Chapter 5

Classical Cryptography

5.1 RSA Algorithm

The RSA algorithm involves three steps:

1. **Key Generation**: RSA involves a public and a private key. The message encrypted with the public key can only be decrypted using the private key. The algorithm for generate the keys is
   (a) Choose two disting prime numbers p, q, with similar bit-length.
   (b) Compute $n = pq$, where n is the modulus for both the public and private keys.
   (c) Compute the *Euler's Totient Function*, $\phi(n) = (p-1)(q-1)$.
   (d) Choose an integer e such that $1 < e < \phi(n)$ and $e, \phi(n)$ are co-primes, $gcd(e, \phi(n)) = 1$.
   (e) e is the public key exponent. $d = e^{-1}(\mod \phi(n))$ is private key exponent. The public key is the modulus n and encryption (expoent) e. The private key is decryption (expoent) d.
2. **Encryption**: Alice transmits the public key (n, e) to Bob, which want to send a message M back to Alice. M is a integer $0 < m < n$, then he compute the ciphertext c as $c = m^e(\mod n)$, and transmit it to Alice.
3. **Decryption**: Alice recover m from c, using her private key expoent d computing $m = c^d(\mod n)$. She recovers M.

Part III

Quantum Information and Computation

Chapter 6

The Advent of the Quantum Computation

6.1 History of Quantum Information and Computation

```
  Any sufficiently advanced
technology is indistinguishable
from magic. (Arthur C. Clarke)
```

In 1985, [DEU85], David Deutsch attempted to define a computation device that would be capable of efficiently simulating a physical system, which means to consider a device to simulate quantum mechanics. Without an answer to this problem, he tried to find out whether it was possible to a quantum computer to efficiently solve computational inefficient problems in a classical computer. In 1994, Peter Shor, [SHO94] demonstrated that the problem of finding the prime factor of an integer, *the discrete logarithmic problem*, could be solved efficiently on a quantum computer, showing that quantum computers are more powerful than Turing machines. In 1995, Lov Grover, [GRO96] provided a *faster* algorithm to database search.

In terms of *information theory*, the famous paper from Claude Shannon, in 1948 [SHA48], defined mathematically the classical concept of information in two theorems: *the noiseless channel coding theorem* (how to store an output from an information source) and the *noisy channel coding theorem* (how much information is possible to transmit through a noisy channel).

Half century later, in 1995, [BEN73], Ben Schumacher[1] gives an analogue to Shannon's theorem for quantum information theory and defines the term qubit as the equivalent to bit.

In quantum computation, a quantum gate of N qubits can be expressed as a vector 2^N dimensional. Quantum gates are unitary transformations that act on just a few qubits at a time.

In 1961, Landauer, [LAND61], claimed that *"Erasure of information is a dissipative/irreversible process"*, it always involves compression of the phase space. The logic gates to perform computation are typically irreversible, for example the NAND gate, where two inputs become output, and the output cannot recover the inputs. One needs at least the thermodynamical threshold, $W = k_B T \ln 2$, to operate the gate.

This conclusion leads to the concept of reversible computation which avoids erasure of the information and in 1973, Bennett, [BEN73], claimed that *Any computation can be formed using only reversible steps, with no dissipation".* Similarly to NAND, but reversible, we can create the *Toffoli gate*, which flips the third bit if the first and second are one. However, this process generates a lot of extra necessary information, which could be reconverted on reversible operations. Today's irreversible computers have dissipation much bigger than the thermodynamical threshold $k_B T \ln 2$ per gate. For future considerations, however, it's important to consider this limit to prevent components from melting.

In 1964, [BE64], Bell's published his famous paper predicting that quantum mechanics cannot be reproduced by any local hidden variable theory. Therefore, quantum information can be encoded in non local correlations between different parts of a physical system.

In classical computation, the required to find the factors p and q on $n = pq$ is believed to be super polynomial in $\log(n)$, for example, $n = 10^{500}$ would be $T(n) = e^{500 \ln 10}$. Therefore the factoring problems was considerable intractable, since it cannot be solved in a time bounded by a polynomial size of the input. However, in 1995, Shor, [SHO94], showed that quantum computing can factor in a polynomial time, $O[(\ln n)^3]$, as we shall see in the next chapters.

Kitaev, Shen and Vyalyi, [KSV02], start their book introducing one of the main motivation on quantum computation: the motivations given by the *computational complexity theory.* Since the time of *Charles Babbage*, comput-

[1] As a friend of mine likes to tell, Ben was a student from Hendrix College.

ers consist of *bits*, which are variables taking values 0 and 1, and a program, which is a sequence of operations using bits. The classical computation is however almost reaching its physical limitation, since we cannot imagine a component or transistor smaller then the size of an atoms, in the order of 1 Angstrom, or 10^{-10} meters, or a clock frequency greater than the frequency of atomic transitions, in the order of 10^{15} Hz.

The history of quantum information and computation started in late 70's, where many techniques for controlling single quantum systems were developed. In the early 80's, Feynman [FEY82] and Deutsch [DEU85], published the ideas of a quantum system to solve a complex computational problem. Deutsch introduced the *Quantum Turing Machine* and then the quantum circuit. A timeline is proposed below.

1970 Landauer, [LAND61], demonstrated importance of reversibility for minimal energy computation.

1973 Stephen Wiesner invents conjugate coding, [WIE73].

1973 Bennett showed the existence of universal reversible Turing machines, [BEN73].

1973 Holevo publishes paper showing thatn qubits cannot carry more than n classical bits of information (Holevo's theorem).

1975 Poplavskii publishes *Thermodynamical models of information processing* (in Russian).

1975 Uspekhi Fizicheskikh Nauk showed the computational infeasibility of simulating quantum systems on classical computers, due to the superposition principle.

1976 Ingarden publishes paper entitled *Quantum Information Theory*, one of the first attempts at creating a quantum information theory, showing that Shannon information theory cannot directly be generalized to the quantum case.

1981 Toffoli-Fredkin designed a universal reversible gate for Boolean logic.

1982 Benioff showed that quantum processes are at least as powerful as Turing machines.

1982 Feynman demonstrated that quantum physics cannot be simulated effectively on classical computers.

1984 Quantum cryptographic protocol BB84 was published, by Bennett and Brassard, for absolutely secure generation of shared secret random classical keys.

1985 Deutsch showed the existence of a universal quantum Turing machine, [DEU85].

1989 First cryptographic experiment for transmission of photons, for distance 32.5cm was performed by Bennett, Brassard and Smolin.

1991 Ekert at the University of Oxford, invents entanglement based secure communication.

1993 Bernstein-Vazirani-Yao showed the existence of an efficient universal quantum Turing machine.

1993 Dan Simon invented an oracle problem for which a quantum computer would be exponentially faster than conventional computer. This algorithm introduced the main ideas for Shor's algorithm.

1993 Quantum teleportation was discovered, by Bennett et al.

1994 Cryptographic experiments were performed for the distance of 10km (using fibers).

1994 Quantum cryptography went through an experimental stage.

1994 Shor discovered a polynomial time quantum algorithm for factorization, [SHO94].

1995 DiVincenzo designed a universal gate with two inputs and outputs.

1995 Cirac and Zoller demonstrated a chance to build quantum computers using existing technologies.

1996 Shor showed the existence of quantum error-correcting codes, [SHO96].

1996 Grover invented the quantum database search algorithm.

1996 The existence of quantum fault-tolerant computation was shown by P. Shor.

1997 Cory, Fahmy and Havel, and at the same time Gershenfeld and Chuang at MIT published the first papers realizing gates for quantum computers based on bulk spin resonance, which the technology based on a nuclear magnetic resonance.

1997 Kitaev described the principles of topological quantum computation as a method for combating decoherence, [KIT97].

1997 Loss and DiVincenzo proposed the Loss-DiVincenzo quantum computer.

1998 First experimental demonstration of a quantum algorithm, solving the Deutsch's problem, by Jones and Mosca.

1998 First working 3-qubit NMR computer.

1998 First execution of Grover's algorithm on an NMR computer.

1999 Braunstein showed that there was no mixed state quantum entanglement in any bulk NMR experiment.

2000 First working 5-qubit NMR computer, first execution of order finding (part of Shor's algorithm), and first working 7-qubit NMR.

2001 First execution of Shor's algorithm.

2001 Linden and Popescu proved that the presence of entanglement is a necessary condition for a large class of quantum protocols.

2001 Knill, Laflamme, and Milburn, launch the field of linear optical quantum computing.

2002 The Potts model and the BMW algebra, by Read.

2003 Pittman and O'Brien demonstrate quantum controlled-not gates using only linear optical elements.

2004 First working pure state NMR quantum computer.

2005 First quantum byte, or qubyte, is created.

2005 Quantum Potts nets, by Fradkin.

2006 New classical loop modes by Jacobsen.

2006 Caging of a qubit in a buckyball and demonstrating of quantum bang-bang error correction.

2006 Search of a database without running a quantum computer.

2006 Braunstein demonstrated the quantum telecloning.

2006 Two dimensional ion trap developed for quantum computing.

2006 Seven atoms placed in stable line, a step on the way to constructing a quantum gate.

2006 Device that can manipulate the up/down spin-states of electrons on quantum dots.

2007 First use of Deutsch's Algorithm in a cluster state quantum computer.

2007 Demonstration of controllably coupled qubits.

2007 Diamond quantum register developed.

2007 Quantum effects demonstrated on tens of nanometers.

2007 Bose-Einstein condensate quantum memory.

2007 The BMW algebra, the chromatic algebra, and the golden identity, with V. Krushkal.

2008 Graphene quantum dot qubits.

2008 Control of quantum tunneling.

2008 Entangled memory developed.

2008 Superior NOT gate developed.

2008 Superior quantum Hall Effect discovered.

2008 Quantum Potts loop models.

2008 Qubit stored for over 1 second in atomic nucleus.

2009 Lifetime of qubits extended to hundreds of milliseconds.

2009 Quantum entanglement demonstrated over 240 microns.

2009 Qubit lifetime extended by factor of 10^3.

2009 Shor's algorithm on a silicon photonic chip.

2009 Google collaborates with D-Wave Systems on image search technology using quantum computing.

2010 Ion trapped in optical trap.

2010 Single electron qubit developed.

6.2 One Qubit

The basic unit of quantum information is the *qubits*, which lives in a Hilbert space $\mathcal{C}^2$, with basis $\{|0\rangle, |1\rangle\}$. The difference between bits and qubits is that a qubit can be in a state other than 0 or 1, but also in a superposition of states. Therefore, a single qubit can be given by a wavefunction

$$|\psi\rangle = A|0\rangle + B|1\rangle$$

and its respective bra $\langle\psi|$. We find $A = \langle 0|\psi\rangle, B = \langle 1|\psi\rangle$, both being the complex amplitudes for finding the particles with spin up or down. If we measure this qubit in the computational basis $|0\rangle, |1\rangle$, the probability of obtaining $|0\rangle$ is AA^* and the probability of obtaining $|1\rangle$ is BB^*. We see that the spatial aspects of these wavefunctions are suppressed, which means that the particles are fixed, such as quantum dots.

Sometimes we can have system defined on other basis besides the previous *computational basis*, such as the familiar states

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

and

$$|-\rangle = \frac{1}{\sqrt{2}}|0\rangle - \frac{1}{\sqrt{2}}|1\rangle,$$

which are orthogonal and normalized [2]. If we want to express $|\psi\rangle$ in this basis, such as $|\psi\rangle = \alpha|+\rangle + |\beta\rangle$, we find α and β as the inner products $\alpha = \langle +|\psi\rangle$ and $\beta = \langle -|\psi\rangle$[3].

If we measure the state $|\psi\rangle$ in the $|+\rangle$ and $|-\rangle$ basis, the probability of getting $|+\rangle$ is $\alpha\alpha^*$ and the probability of getting $|-\rangle$ is $\beta\beta^*$.

The Bloch Sphere

One useful way of thinking about qubits is in a geometric representation called *Bloch sphere*. Since $|A|^2 + |B|^2 = 1$, we can rewrite our superposition state as

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

[2] $\langle +|-\rangle = 0$ and $\langle \pm|\pm\rangle = 1$.

[3] We can prove it using explicitly the orthonormality of the basis.

6.3 Two Qubits

We can write a two qubit wavefunction as $|\psi_{12}\rangle = |00\rangle+|01\rangle+|10\rangle+|11\rangle$ which are the tensorial representation of two qubits of the form $|\phi_1\rangle = a_1|0\rangle + b_1|1\rangle$ and $|\phi_2\rangle = a_2|0\rangle + b_2|1\rangle$,

$$|\phi_1\rangle \otimes |\phi_2\rangle = a_1a_2|00\rangle + a_1b_2|01\rangle + a_2b_1|10\rangle + b_1b_2|11\rangle.$$

Qubits Evolution

The manipulation of a qubit is given by the unitary 2×2 matrices U, which is a linear combination of the Pauli matrices. The unitary operators, or *gates*, manipulate the qubit states. Being unitary allows we calculate the quantum evolution of our wavefunction $|\psi\rangle$: the new state will be $|\psi'\rangle = U|\psi\rangle$.

A *Hadamard matrix* is a square matrix whose entries are either $+1$ or 1 and whose rows are mutually orthogonal. The Hadamard gate is a reflection about the line $\theta = \pi/8$. A Hadamard matrix H of order n satisfies

$$HH^T = nI_n. \tag{6.3.1}$$

We express the two qubit unitary $H \otimes I$ or $I \otimes H$[4] in terms of the basis $|00\rangle, |01\rangle, |10\rangle$, and $|11\rangle$, which is a 4×4 matrix. The evolution of $|\psi_{12}\rangle$ is given by $|\psi'_{12}\rangle = (H \otimes I)|\psi_{12}\rangle$.

Let us write

$$-\boxed{H}- = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix}$$

Applying $H \otimes H$ to $|\psi_{12}\rangle$

$$H \otimes H|\psi_{12}\rangle = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} = |00\rangle$$

Therefore the probability of getting $|00\rangle$ is one and zero for the other three states.

[4] $H \otimes I$ and $I \otimes H$ commute.

6.3.1 Bell States

The *Bell basis*, or *EPR pair*, is as set of orthonormal four 2-qubit wavefunction $|00\rangle + |11\rangle$. In general, they can be written as

$$|\Psi_+\rangle = \frac{1}{\sqrt{2}}\Big(|01\rangle + |10\rangle\Big), |\Psi_+\rangle = \frac{1}{\sqrt{2}}\Big(|01\rangle - |10\rangle\Big), \tag{6.3.2}$$

$$|\Phi_+\rangle = \frac{1}{\sqrt{2}}\Big(|00\rangle + |11\rangle\Big), |\Phi_+\rangle = \frac{1}{\sqrt{2}}\Big(|00\rangle - |11\rangle\Big). \tag{6.3.3}$$

We can rearrange in our previous basis as

$$|00\rangle = \frac{1}{\sqrt{2}}\Big(|\Phi_+\rangle + |\Phi_-\rangle\Big), \tag{6.3.4}$$

$$|01\rangle = \frac{1}{\sqrt{2}}\Big(|\Psi_+\rangle + |\Psi_-\rangle\Big), \tag{6.3.5}$$

$$|10\rangle = \frac{1}{\sqrt{2}}\Big(|\Psi_+\rangle - |\Psi_-\rangle\Big), \tag{6.3.6}$$

$$|11\rangle = \frac{1}{\sqrt{2}}\Big(|\Phi_+\rangle - |\Phi_-\rangle\Big). \tag{6.3.7}$$

The two-qubit evolution matrix U has as columns $\Phi_+, \Psi_+, \Phi_-, \Psi_-$ and the rows are the computational basis. To perform a measurement in a different basis than the computational basis, we use the unitary evolution followed by a measurement in the computational basis, i.e. we find

$$U^\dagger|\psi\rangle = \begin{bmatrix} \langle\Phi_+| \\ \langle\Psi_+| \\ \langle\Phi_-| \\ \langle\Psi_-| \end{bmatrix} |\psi\rangle = \begin{bmatrix} \langle\Phi_+|\psi\rangle \\ \langle\Psi_+|\psi\rangle \\ \langle\Phi_-|\psi\rangle \\ \langle\Psi_-|\psi\rangle \end{bmatrix}$$

The Bell states has a central role in quantum teleportation and superdense coding, as we shall see soon. After we measure the first qubit, the result of the second qubit will always give the same result as the first qubit, a typical quantum correlation.

6.4 Three to n-Qubits

6.4.1 GHZ State

The *Greenberger-Horne-Zeilinger state* is a type of *entangled* quantum state which involves at least three subsystems. It has the general form

$$|GHZ\rangle = \frac{|0\rangle^{\otimes M} + |1\rangle^{\otimes M}}{\sqrt{2}}. \tag{6.4.1}$$

Therefore, for three-qubit entangled wavefunction we have

$$|GHZ\rangle = \frac{|000\rangle + |111\rangle}{\sqrt{2}}. \tag{6.4.2}$$

Projectors and Probabilities

Let us calculate the probability of the wavefunctions on $|000\rangle, |111\rangle$, measuring the first qubit in the computational basis$|0\rangle$ or $|1\langle$. For this purpose we use the projectors

$$P_0 = |0\rangle\langle 0|, P_1 = |1\rangle\langle 1|, \tag{6.4.3}$$

and for three-qubits

$$\begin{aligned} P_0 \otimes I \otimes I &= \Big(|0\rangle\langle 0|\Big) \otimes \Big(|0\rangle\langle 0| + |1\rangle\langle 1|\Big) \otimes \Big(|0\rangle\langle 0| + |1\rangle\langle 1|\Big), \\ &= |000\rangle\langle 000| + |001\rangle\langle 001| + |010\rangle\langle 010| + |011\rangle\langle 011|, \\ P_1 \otimes I \otimes I &= \Big(|1\rangle\langle 1|\Big) \otimes \Big(|0\rangle\langle 0| + |1\rangle\langle 1|\Big) \otimes \Big(|0\rangle\langle 0| + |1\rangle\langle 1|\Big), \\ &= |100\rangle\langle 100| + |101\rangle\langle 101| + |110\rangle\langle 110| + |111\rangle\langle 111|. \end{aligned}$$

Applying the projectors into the GHZ state we have

$$\begin{aligned} (P_0 \otimes I \otimes I)|GHZ\rangle &= \frac{1}{\sqrt{2}}|000\rangle, \\ (P_1 \otimes I \otimes I)|GHZ\rangle &= \frac{1}{\sqrt{2}}|111\rangle. \end{aligned}$$

To find the probabilities,

$$\begin{aligned} Pr(0) &= \langle GHZ|(P_0 \otimes I \otimes I)|GHZ\rangle \\ &= \frac{1}{2}\langle 000|000\rangle, \\ &= \frac{1}{2}, \\ Pr(1) &= \langle GHZ|(P_1 \otimes I \otimes I)|GHZ\rangle \\ &= \frac{1}{2}\langle 111|111\rangle \\ &= \frac{1}{2}. \end{aligned}$$

Projectors and Probabilities and Entanglement

We now want to measure to measure the first qubit in the basis $|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ and $|-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$. The projectors are

$$\begin{aligned} P_+ &= |+\rangle\langle +|, \\ &= \frac{1}{\sqrt{2}}\Big(|0\rangle\langle 0| + |0\rangle\langle 1| + |1\rangle\langle 0| + |1\rangle\langle 1|\Big), \\ P_- &= |-\rangle\langle -|. \\ &= \frac{1}{\sqrt{2}}\Big(|0\rangle\langle 0| - |0\rangle\langle 1| - |1\rangle\langle 0| + |1\rangle\langle 1|\Big). \end{aligned}$$

For three-qubits

$$\begin{aligned} P_+ \otimes I \otimes I &= \Big(|0\rangle\langle 0| + |0\rangle\langle 1| + |1\rangle\langle 0| + |1\rangle\langle 1|\Big) \otimes \Big(|0\rangle\langle 0| + |1\rangle\langle 1|\Big) \otimes \Big(|0\rangle\langle 0| + |1\rangle\langle 1|\Big), \\ &= \frac{1}{2}\Big[|000\rangle\langle 000| + |001\rangle\langle 001| + |010\rangle\langle 010| + |011\rangle\langle 011| + \\ &+ |000\rangle\langle 100| + |001\rangle\langle 101| + |010\rangle\langle 110| + |011\rangle\langle 111| + \\ &+ |100\rangle\langle 000| + |101\rangle\langle 001| + |110\rangle\langle 010| + |111\rangle\langle 011| + \\ &+ |100\rangle\langle 100| + |101\rangle\langle 101| + |110\rangle\langle 110| + |111\rangle\langle 111|\Big], \end{aligned}$$

and

$$\begin{aligned}
P_- \otimes I \otimes I &= \Big(|0\rangle\langle 0| - |0\rangle\langle 1| - |1\rangle\langle 0| + |1\rangle\langle 1|\Big) \otimes \Big(|0\rangle\langle 0| + |1\rangle\langle 1|\Big) \otimes \Big(|0\rangle\langle 0| + |1\rangle\langle 1|\Big), \\
&= \frac{1}{2}\Big[|000\rangle\langle 000| + |001\rangle\langle 001| + |010\rangle\langle 010| + |011\rangle\langle 011| - \\
&- |000\rangle\langle 100| - |001\rangle\langle 101| - |010\rangle\langle 110| - |011\rangle\langle 111| - \\
&- |100\rangle\langle 000| - |101\rangle\langle 001| - |110\rangle\langle 010| - |111\rangle\langle 011| + \\
&+ |100\rangle\langle 100| + |101\rangle\langle 101| + |110\rangle\langle 110| + |111\rangle\langle 111|\Big].
\end{aligned}$$

The probabilities are

$$\begin{aligned}
Pr(+) &= \langle GHZ|(P+ \otimes I \otimes I)|GHZ\rangle, \\
&= \frac{1}{2}, \\
Pr(-) &= \langle GHZ|(P_- \otimes I \otimes I)|GHZ\rangle, \\
&= \frac{1}{2}.
\end{aligned}$$

Clearly we see that in this basis, the second and third qubits are entangled after the measurement.

Measuring all Three Qubits

To measure all three qubits in the $|+\rangle, |-\rangle$ basis we calculate the tensor product of three projectors, $P_A \otimes P_B \otimes P_C$. Most terms will be canceled in the inner product with $|GHZ\rangle$, the only terms that survives are

$$P_A \otimes P_B \otimes P_C \propto \Big(|000\rangle\langle 000| \pm |000\rangle\langle 111| \pm |111\rangle\langle 111| \pm ...\Big)$$

The probabilities of the eight possible outcomes will depend on the $\pm$ and are calculated making $\langle GHZ|P_A \otimes P_B \otimes P_C|GHZ\rangle$.

6.4.2 n Qubits

A system of n-qubits is a finite dimensional Hilbert space of dimension 2^n. We can represent the n qubits with the wavefunction

$$|\phi\rangle = \frac{1}{\sqrt{2^n}} \sum_{x=0}^{2^n-1} |x\rangle.$$

6.5 Quantum Gates and Quantum Circuits

6.5.1 One Qubit

Classical computer circuits are composed of wires, which transport information, and logic gates, which make conversion of information. In quantum computation the quantum gates represent *unitary* matrices that act on the states. For qubit defined as

$$|\psi\rangle = \begin{bmatrix} A \\ B \end{bmatrix},$$

the quantum **NOT** gate can be represented as

$$-\boxed{X}- = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix},$$

and it swaps the 0 to 1 and 1 to 0. Other important two gates are **Z** and **Hadamard**,

$$-\boxed{Z}- = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix},$$

and

$$-\boxed{H}- = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix},$$

which is the square-root of the NOT gate.

6.5.2 n-Qubits

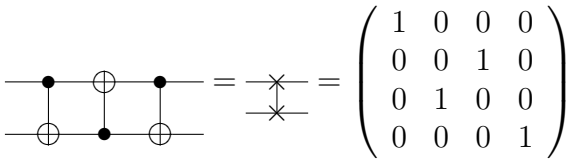
In classical computation, the **NAND** gate is called universal gate since any function on bits can be computed from the composition of this gate (what does not happen for NOT or XOR, for example). Thy also are *non-invertible, irreversible.*

In quantum computation, the unitary quantum gates are always invertible. The universal quantum gate is the *controlled-NOT*. The **CNOT** gate has two input qubits, one is the *control* and the other is the *target* qubit. If the control qubit is 1, the target qubit is flipped,

$$\begin{array}{l} |A\rangle \\ |B\rangle \end{array} \quad \begin{array}{c} \bullet \\ \oplus \end{array} \quad \begin{array}{l} |A\rangle \\ |A \oplus B\rangle \end{array}$$

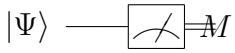
$$U_{CNOT} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

A circuit that swaps the states of two qubits can be written as



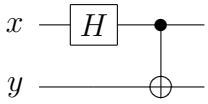
$$= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

The measurement of a quantum circuit converts a qubit state to a classical bit M, with some probability,



6.5.3 A Circuit for Bell States

We can construct a circuit with input any computational basis, $|00\rangle, |10\rangle, |01\rangle$ or $|11\rangle$, to output Bell states by joining a Hadamard and a CNOT gate,



producing

IN	OUT
$\|00\rangle$	$\frac{(\|00\rangle+\|11\rangle)}{\sqrt{2}}$
$\|01\rangle$	$\frac{(\|01\rangle+\|10\rangle)}{\sqrt{2}}$
$\|10\rangle$	$\frac{(\|00\rangle-\|11\rangle)}{\sqrt{2}}$
$\|11\rangle$	$\frac{(\|01\rangle-\|10\rangle)}{\sqrt{2}}$

Example: Quantum Teleportation

Let us study a simple case of quantum teleportation (or the EPR paradox) from our Bells states and what we know from quantum circuits.

1. Suppose A and B generated in the past an EPR pair, each taking one qubit, and keeping their qubit when they separated.

2. In the present, A wants to deliver a quibit $|\psi\rangle$ to B and she doesn't know the state of this qubit (nether can she copies it because of the no-cloning theorem). She only can send classical information to B.

3. By quantum computation, A can use the entangled EPR pair to send $|\psi\rangle$ to B, with very small classical communication. The heuristic description of the process is

   (a) A interacts $|\psi\rangle$ to her half of the EPR pair.

   (b) A resumes the two quibits, obtaining 00, 01, 10 or 11.

   (c) A sends the information to B.

   (d) Depending on A's message, B performs one of four operations on his half EPR and recover $|\psi\rangle$

4. In mathematical description, the problems can represented by

   (a) The state to be teleported is $|\psi\rangle = A|0\rangle + B|1\rangle$. Supposing their EPR state is $|00\rangle + |11\rangle$The input in the circuit is

   $$|\psi_0\rangle = |\psi\rangle|EPR\rangle = \frac{1}{\sqrt{2}}\Big[A|0\rangle(|00\rangle + |11\rangle) + B|1\rangle(|00\rangle + |11\rangle)\Big],$$

   where only the third qubit belongs to B.

   (b) A sends her state to a CNOT gate,

   $$|\psi_1\rangle = \frac{1}{\sqrt{2}}\Big[A|0\rangle(|00\rangle + |11\rangle) + B|1\rangle(|10\rangle + |01\rangle)\Big].$$

   (c) Then she sends to a Hadamard gate,

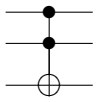
   $$|\psi_2\rangle = \frac{1}{\sqrt{2}}\Big[A(|0\rangle + |1\rangle)(|00\rangle + |11\rangle) + B(|0\rangle - |1\rangle)(|10\rangle + |01\rangle)\Big],$$

   which giver four terms and gives the four possibility of measurements by A. The first two qubits are from A and the last quibit will be B's state.

(d) Depending on this outcome, B's qubit will be one of these four possible states. Knowing A's result, B can recover $\psi\rangle$ by applying the appropriate gate. For example, if A measures 01, B applies X gate to recover 00 (which we've used in this example). What prevents the fact that information travels faster than light is that for B find his outcome, he needs to know A's measurement.

Example: Quantum Toffoli Gate

The Toffoli gate can be used as a quantum logic gate, permutating the basis in the same way as the classical version.



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

Chapter 7

Entanglement

Chapter 8

Quantum Circuits

8.1 Reversible Classical Computation

8.2 Stony Brook: Likharev's First Computer Model based on Electronic Devices

8.3 Precision

8.4 Universal Gate Sets

Chapter 9

Quantum Algorithms

9.1 Quantum Parallelism

In 1985, [DEU85], Deutsch stated that *"Quantum computation can best realize its computational potential by invoking quantum pararelism"*.

Quantum parallelism is one of the principal characteristics of many quantum algorithms, allowing quantum computers to evaluate a function $f(x)$ for many values of x at the same time. The steps are the following:

1. We consider the input states

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

and

$$|0\rangle.$$

2. We apply a transformation U_f that will result on the output state

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

which contains information about both $f(0)$ and $f(1)$.

3. Quantum parallel evaluation of a function with an n bit input x and 1 bit output, $f(x)$, can be performed by preparing $n+1$ qubit states

$|0\rangle^{\otimes n}|0\rangle$, and then applying Hadarmard transformations ($H^{\otimes n}$) to the first n qubits, followed by U_f. We end up getting the state

$$\frac{1}{\sqrt{2^n}} \sum_x |x\rangle|f(x)\rangle.$$

9.2 The Class BQP

9.3 Grover's Search Algorithm

9.4 Lower Bounds for Blackbox Problems

9.5 Simon's and Shor's Algorithms

9.6 Phase Estimation

9.7 Quantum Fourier Transform

Chapter 10

Fault-Tolerant Quantum Computation

The Physical realization of a quantum computer is a big challenge. One open problems is *decoherence*, which is the non local correlations of the environment to our quantum system, and systematic errors in unitary transformations. Quantum gates form a continuum, $U = U_0(1 + O(\epsilon))$. In classical computers, the errors are attenuated by cooling, but this process is not suitable in quantum computation.

The type of errors in quantum computation are:

- Phase Errors: $|0\rangle \rightarrow |1\rangle$ and $|0\rangle \rightarrow -|0\rangle$.
- Small Errors: By a small ϵ in the continuous state $A|0\rangle + B|1\rangle$.
- Disturbance by Measurement.
- No-Cloning.

One of the most important contributions on fault-tolerant quantum computation was given by P. Shor, [SHO96], in 1996, when he discovery the fault-tolerant quantum computation: *an arbitrary quantum circuit can be simulated using imperfect gates, provided that these gates are close to the ideal ones up to a constant precision* δ. Many following references reproduce what he discovered in that paper.

```
For any quantum computation with t gates, we show how to
build a polynomial size quantum circuit that tolerates O(1/ log^c t)
```

> amounts of inaccuracy and decoherence per gate, for some constant c; the previous bound was O(1/t). We do this by showing that operations can be performed on quantum data encoded by quantum error-correcting codes without decoding this data.
> (P. Shor, 1996)

The Shor's quantum error-correcting code can be summarized as following:

Chapter 11

Quantum Cryptography

Chapter 12

Entropy and Information

Chapter 13

The Reality of a Quantum Computer

A first necessary condition for the construction of a quantum computer is the reversibility: transition function mapping states to their successors at a given later time should be one-to-one, with no increase in physical entropy. The only potential way to improve the energy efficiency of computers beyond the fundamental von Neumann-Landauer limit $k_B T \ln(2)$, energy dissipated per irreversible bit operation.

One of the main problems is the decohrence, which is irreversible/non-unitary. Any operation must be quicker than the decoherence times. If the error rate is small enough we can use a quantum error correction algorithm.

There are already many approaches for the realizaton of a quantum computer,

- Superconductor-based quantum computers (including SQUID-based quantum computers), [AVE08].
- Trapped ion quantum computer.
- Optical lattices.
- Topological quantum computer, [FKLW02].
- Quantum dot on surface (e.g. the Loss-DiVincenzo quantum computer).
- Nuclear magnetic resonance.

- Cavity quantum electrodynamics (CQED)

13.1 Concepts on Solid State

13.2 Concepts on Electronics

Clock Rate Rate in bits per second, given in hertz. A single clock cycle goes between a logical zero and a logical one state. For classical computation, the clock of a CPU is normally determined by the frequency of an oscillator crystal. The clock rate is only one of several factors that can influence performance when comparing processors. Nowadays: the limits to energy per transition are explored by reversible computing (not yet implemented). CPU faster than 3.5 GHz is limit to thermodynamic limits in current semiconductor process. In 2010 the fasted clock speed microprocessor was $z196$, with 5.2 GHz.

Shunt Resistors Allows electric current to pass around another point in the circuit.

13.3 Universal Adiabatic Quantum Computer

13.3.1 The Adiabatic Theorem

The adiabatic theorem to calculations:

- Complex Hamiltonian in the ground state.
- System with simple Hamiltonian initialized on ground state.
- Simple hamiltonian is adiabatically evolved to the complex hamiltonian.
- Theorem: system remains in the ground state.
- Get over of decoherence since system is in ground state (keeping temperature of bath lower).

13.4 Trapped Ions

Quantum state of each ion is a linear combination of the ground state and a long-lived metastable excited state. A coherent linear combination of two levels

$$A|0\rangle + Be^{i\omega t}|1\rangle,$$

can survive $t \gg \tau$ excited states. The spontaneous decay is the dominant form of decoherence.

The main difficult of this approach is to get two qubits interacting, and the slow processing ($\sim$ 100 kHz).

13.5 Nuclear Magnetic Resonance

Qubits are carried by certain nuclear spin in a particular molecule, with a constant magnetic field. Gates are implemented as the dipole-dipole interactions.

This method can be used to prepare an entangled state of 3 qubits.

13.6 Superconductor-based Quantum Computers

13.6.1 Josephson effect

Standard measure of voltage. Two superconductors separated by a thin insulating layer can have tunneling of Cooper pairs of electrons through the junction. The Cooper pairs on each side of the junction can be represented by a wavefunction similar to a free particle (exponential). In the D.C. Josephson effect, the current is proportional to the phase difference of the wavefunctions and can exists in the junction in the absence of voltage.

In A.C., the Josephson junction oscillates with a characteristic frequency proportional to V,

$$f = \frac{2e}{h}V.$$

The A.C. Josephson effect is a voltage-to-frequency converter.

13.6.2 SQUID

A Superconducting Quantum Interference Device is one of the most sensitive detector for magnetic field. It can be used to the implementation of quantum entanglement between a SQUID-qubit and a spin-qubit.

Flux Qubit A persistent current qubit is micro-sized loops of superconducting metal interrupted by Joseph junctions. In the computer basis states it is the circulating current clockwise or anti-clockwise. They are multiples of the quantum flux unit. The Andreev interferometer probes the flux qubits.

Charge Qubit Superconducting qubit whose basis states are charge states (presence or absence of cooper pairs).

Phase Qubit First quantum machine last year.

Chapter 14

Topological Quantum Computation

```
   A 2D quantum system with anynioc excitations can be
considered as a quantum computer. Unitary transformations
  can be performed by moving the excitations around each
other. Measurements can be performed by joining excitations
in pairs and observing the result of fusion. Such computation
     is fault-tolerant by its physical nature. (Kitaev, 2008)
```

The idea of topological quantum computation is based on 2D anyons, where the world lines cross over one another to form braid in 3D. *Braids* form the logic gates to the computer and they are much more stable than trapped quantum particles. Important papers in the subject on these aspects were

- Kitaev, Fault-tolerant quantum computation by anyons (1997), [KIT97].
- Preskill and Ogburn, Topological quantum computation (1997).
- Preskill, Fault-tolerant quantum computation (1997).
- Mochon, Anyons from non-solvable groups are sufficient for universal quantum computation (2003).
- Mochon, Anyon computers with smaller groups (2004).
- Freedman, Larsen, and Wang, A modular functo rwhich is universal for quantum computation (2000).

- Freedman, Kitaev, and Wang, Simulation of topological field theories by quantum computers (2000).

A *topologically ordered state* has a non-local quantum entanglement. The pattern of quantum entanglements cannot be destroyed by local perturbations, reducing the effect of decoherence, and the information may last longer.

14.1 Topology of Anyons

A *Quantum Group* denotes various kinds of noncommutative algebra with additional structure. In general, a quantum group is some kind of *Hopf algebra*.

14.2 Abelian Anyons

Abelian anyon models can also be used for robust quantum memory.

14.3 Non-Abelian Anyons

A model of anyons is a theory of a two-dimensional medium with a mass gap, where the particles carry locally conserved charges. We define the model by specifying:

- A finite list of particle labels (a,b,c,). These indicate the possible values of the conserved charge that a particle can carry. If a particle is kept isolated from other particles, its label never changes.
- Rules for fusing (and splitting). These specify the possible values of the charge that can result when two charged particles are combined.
- Rules for braiding. These specify what happens when two neighboring particles are exchanged (or when one is rotated by 2π).

Appendix A

Mathematical Formulae

Quantum Mechanics

$\partial_t(g^{-1}) = -g^{-1}(\partial_t g)g^{-1}$
The spectrum of a operator $S^2 = 1$ is $s = \pm 1$
The spectrum of a operator $T^3 = 1$ is $t = 1, e^{\frac{\pm 2\pi i}{3}}$

$$e^A e^B = exp(A + B + \frac{1}{2}[A, B] + \frac{1}{12}([A, [A, B]]...)$$

Gaussian Integral

$$\int_\infty^\infty e^{-ax^2} = \sqrt{\frac{\pi}{a}}$$
$$\int_\infty^\infty x^2 e^{-ax^2} = \frac{1}{2a}\sqrt{\frac{\pi}{a}}$$

Delta Function

$$\int_{\infty}^{\infty} f(x)\delta(x-a)dx = f(a)$$
$$\delta(x-a) = 0 \text{ for } a \neq x$$
$$\delta(ax) = \frac{1}{|a|}\delta(x)$$
$$\delta(x^2-a^2) = \frac{1}{|a|}(\delta(x+a)+\delta(x+a))$$
$$\delta(g(x)) = \sum_i \frac{\delta(x-x_i)}{g'(x_i)}$$
$$x\delta'(x) = -\delta(x)$$
$$\delta(x^2+x-2) = \delta((x-1)(x+2))$$
$$\int f(x)\delta^n(x)dx = -\int \frac{\partial f}{\partial x}\delta^{n-1}dx$$
$$x^n\delta^n(x) = (-1)^n n!\delta(x)$$
$$\int f(x)\delta'(x-a)dx = -f'(a)$$
$$\int_1^1 \delta(\frac{1}{x})dx = 0$$
$$\frac{\eta}{\eta^2+x^2} \to \pi\delta(x), \text{ when } \eta \to 0.$$

The Fourier expansion:

$$\begin{aligned}\delta(x-a) &= \frac{1}{2\pi} + \frac{1}{\pi}\sum_{n=1}^{\infty}(cos(na)cos(nx) + sin(na)sin(nx)) \\ &= \frac{1}{2\pi} + \frac{1}{\pi}\sum_{n=1}^{\infty} cos(n(x-a))\end{aligned}$$

A.1 Important Relations

$$M = e^A = 1 + A + \frac{A^2}{2}...$$

$$M = \text{ Lim}_{N\to\infty}\left(1 + \frac{A}{N}\right).$$

$$\ln(\det \text{ M}) = \text{tr (Ln M)}.$$

$$\det B = \prod_i b_i = e^{\sum_i \log b_i} = e^{\text{ tr (log B)}}.$$

Appendix B

Notations Used in the References

We shall call Kitaev and Shen and Vyalyi's book, [KSV02], as **KSV**; Nielsen and Chuang's book, [NC00], as **NC**; and Preskill's notes, [PRES01], as **PR**.

Symbols

SYMBOL	KSV	NC	PR
LOGICAL OR	$\vee$		
LOGICAL AND	$\wedge$		
NEGATION	$\neg$		
ADDITION MOD 2	$\oplus$		
TRANSITION FUNCTION (Turing Machine)	$\delta(.,.)$		
A IMPLIES B	$A \Rightarrow B$		
A IS LOGICALLY EQUIV TO B	$A \Leftrightarrow B$		
n-th TENSOR OF DEGREE O $\mathcal{M}$	$\mathcal{M}^{\otimes n}$		
OPERADOR U TO A QUANTUM REGISTER	$U[A]$		
CLASSICAL BIT	$\mathbb{B}$		
QUANTUM BIT	B		
FINITE FIELD Of q ELEMENTS	$\mathbb{F}_q$		

Matrices and Circuits

Measurement

Hadamard

$$= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

Pauli-X

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

Pauli-Y

$$= \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

Pauli-Z

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

Phase

$$= \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}$$

$\pi/8$

$$= \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}$$

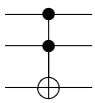
CNOT

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

SWAP

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

Toffoli



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

Complexity Symbols

COMPLEXITY CLASSES	References in the Notes
NC	4.3.2
P	4.3.1
BPP	**??**
P/POLY	**??**
NP	4.3.2
BQP	4.3.4
NQNP	**??**
PSPACE	4.3.3
EXPTIME	**??**

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