Handbook

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Abstract

Somewhat syntetic summaries of courses whose exams I had to prepare. Green boxes are for missing or as of yet unclear parts, blue boxes are for personal additions.

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Chapter 1

Quantum Mechanics

1.1 Definitions

Spectrum (of an observable $\hat{A}$): it is the set of values we can obtain by measuring it, denoted as $\sigma(\hat{A}) \subseteq \mathbb{R}$.

$$\sigma(A) = \left\{ a \in \mathbb{R} : \inf_{\psi \in D(A)} \Delta A_{a,\psi} = 0 \right\} \tag{1.1.1}$$

where $0 \in D(A)$ is not considered when computing the infimum.

Continuous and discrete The *discrete spectrum* $\sigma_d(A)$ is the subset of $\sigma(A)$ of all the a such that $\exists \psi : \Delta A_{a,\psi} = 0$. It is always countable because of the separability of the space. The *continuous spectrum* $\sigma_c(A)$ consists of its complementary in $\sigma(A)$.

Mathematical definition The spectrum of an operator A can be alternatively defined as:

$$\sigma(A) = \left\{ a \in \mathbb{C} : (A - a\mathbb{1})^{-1} \notin \mathcal{B}(\mathbb{R}^n) \right\} \tag{1.1.2}$$

And we have:

1. The discrete spectrum, where there exists an eigenvector for A corresponding to a;
2. The continuous spectrum, where $A - a\mathbb{1}$ can be inverted in a dense domain, but its inverse is unbounded;
3. The residual spectrum, where neither condition holds ($A - a\mathbb{1}$ is not invertible in a dense domain).

Pure State Maximal information about a system.

Expectation value It is the (arithmetic) average we would get by repeatedly performing the same measurement of the observable $\hat{A}$ on the same system in the state Σ, in the limit of $N \to \infty$ measurements, denoted as $\langle \hat{A} \rangle_\Sigma$.

Lebesgue-Stieltjes Measure It is a function $\mu : \mathcal{B}(\mathbb{R}) \to \mathbb{R}$ such that $\mu(\emptyset) = 0$, and which is countably additive. We use the measure denoted by $\mu = \mathrm{d}g$, with g a real positive function, defined by:

$$\mu\big(]a, b[\big) = \lim_{\varepsilon \to 0} g(b - \varepsilon) - g(a + \varepsilon) \tag{1.1.3}$$

With this we define the Lebesgue integral as usual, getting

$$\int f \,\mathrm{d}g = \int f \frac{\mathrm{d}g}{\mathrm{d}\lambda} \,\mathrm{d}\lambda \tag{1.1.4}$$

where the derivative of g is to be interpreted in a distributional sense.

Probability measure If we have an observable $\hat{A}$ and a state Σ, the function $\mathrm{d}P_\Sigma^A(\lambda)$ is the one given by applying the Riesz-Markov theorem to the linear functional $g \to \langle g(A) \rangle_\Sigma$, such that:

$$\langle A \rangle_\Sigma = \int g(\lambda) \,\mathrm{d}P_\Sigma^A(\lambda) \tag{1.1.5}$$

With the help of equation (1.4.2) we then define

$$P_\Sigma^A(\lambda) = \langle \Theta(\lambda - A) \rangle_\Sigma \tag{1.1.6}$$

Abstract probability measure $P^A(\lambda) = \Theta(\lambda - A)$. It allows us to abstract from equation (1.1.6), having

$$f(A) = \int f(\lambda) \,\mathrm{d}P^A(\lambda) \tag{1.1.7}$$

Fluctuations of an observable $\hat{A}$ around a value a:

$$(\Delta A)^2_{\Sigma,a} = \langle (\lambda - a)^2 \rangle_\Sigma = \int (\lambda - a)^2 \,\mathrm{d}P_\Sigma^A(\lambda) \tag{1.1.8}$$

We usually take the fluctuations around the expected value, and define $\Delta A_{\Sigma, \langle A \rangle_\Sigma} = \Delta A_\Sigma$.

Eigenstate A state ψ such that the fluctuations around the expected value satisfy:

$$\inf_{\psi \in D(A)} \Delta A_\psi = 0 \tag{1.1.9}$$

. $\langle A \rangle_\Sigma = a$ is the corresponding eigenvalue. We use λ to represent the eigenvalue, $|\lambda\rangle$ to represent the eigenstate.

Vector ray A subset of the Hilbert space containing vectors in the form $e^{i\alpha}\psi$, for a fixed $\psi \in \mathcal{H}$ and a varying $\alpha \in \mathbb{R}$.

L^2 it is the space of square-integrable complex-valued functions, modulo equality almost everywhere. It is a Hilbert space.

Abstract Hilbert space Since every Hilbert space is isometrically isomorphic to ℓ_2, we say that $|\psi\rangle$ is in an abstract space, and $\psi(x) = \langle x|\psi\rangle$, $\tilde{\psi}(p) = \langle p|\psi\rangle$ are *representations*.

Linear functionals They take a vector ψ in $\mathcal{H}$ and return a complex number. The norm of a functional F is:

$$\|F\| = \sup_{\|\psi\|=1} F(\psi) < \infty \tag{1.1.10}$$

They belong to the dual of the Hilbert space, $\mathcal{H}^*$, as the application of F to ψ can always, by Riesz-Fischer, be written as $\langle\phi|\psi\rangle$, with $\|\phi\|_{\mathcal{H}} = \|F\|_{\mathcal{H}^*}$. Note: the functionals act on $\mathcal{H}$, not directly on $\mathcal{H}/\mathbb{C}_0$.

Distance in $\mathcal{H}/\mathbb{C}_0$ It is defined by:

$$d\Big(|\psi\rangle, |\phi\rangle\Big) = \left(1 - \frac{\Big|\langle\psi|\phi\rangle\Big|^2}{\|\phi\|^2\|\psi\|^2}\right)^{1/2} \tag{1.1.11}$$

Adjoint of an operator The adjoint $A^\dagger$ of an operator A is defined by $\langle\phi|A\psi\rangle = \Big\langle A^\dagger\phi\Big|\psi\Big\rangle$, with domain $D(A^\dagger)$ containing all $\phi \in \mathcal{H}$ such that:

$$\sup_{\substack{\psi\in D(A)\\ \|\psi\|=1}} \Big|\langle\phi|A\psi\rangle\Big| < \infty \tag{1.1.12}$$

Symmetric operators An operator A is symmetric if $D(A^\dagger) \supseteq D(A)$ and, in $D(A)$, $A = A^\dagger$.

Self-adjoint operators A symmetric operator A is self-adjoint if $D(A) = D(A^\dagger)$.

Projectors Operators P such that $P^2 = P$ and $P = P^\dagger$. For every vector there is a projector $|\psi\rangle\langle\psi|$.

Unitary operators Operators U such that $UU^\dagger = U^\dagger U = \mathbb{1}$.

Spectral Family It is a one-parameter family of operators $P(\lambda)$, $\lambda \in \mathbb{R}$, such that:

1. $\forall\lambda$: $P(\lambda)$ is a projector;
2. $\lim_{\lambda\to+\infty} P(\lambda) = \mathbb{1}$ and $\lim_{\lambda\to-\infty} P(\lambda) =$;
3. $P(\lambda)P(\mu) = P(\min\{\lambda, \mu\})$;
4. $\lim_{\lambda\to\mu^+} P(\lambda) = P(\mu)$.

Probability density function Given a concrete probability measure $\mathrm{d}P^A_\psi(\lambda)$ we define its pdf as:

$$W^A_\psi(\lambda) = \frac{\mathrm{d}P^A_\psi(\lambda)}{\mathrm{d}\lambda} \tag{1.1.13}$$

this derivative is generally to be understood in a distributional sense: the probability measure can be discotinuous.

Gelfand Triple Given an operator A, we want to represent the eigenvectors corresponding to its continuous spectrum, which do not belong to $\mathcal{H}$. So we take a subset of $\mathcal{H}$, such that:

1. $\Phi_A \subseteq D(A)$;
2. $\overline{\Phi_A} = \mathcal{H}$;
3. A is continuous (ie bounded) on Φ_A wrt Φ_A's topology;
4. Φ_A is nuclear: if we have two continuous linear operators in the cartesian product of Φ_A with itself, then we can combine them into a continuous operator in the tensor product of Φ_A with itself.

On generalized eigenvectors If a is in the continuous spectrum of A, we can still write an eigenvalue equation as $AF_a = aF_a$; but F_a will belong to Φ_A^*. Of course this is just formal, and it is understood to mean that $AF_a(\phi) = F_a(A\phi)$ holds $\forall \phi \in \Phi_A$.

On generalized autobras In Dirac notation, we define a generalized autobra $\langle\lambda| \in \Phi_A^*$ of A by $\langle\lambda|\phi\rangle = \langle\phi|\lambda\rangle^*$, which is well-defined because it is the scalar product of elements of $\mathcal{H} \supseteq \Phi_A \ni |\lambda\rangle$.

Mixed State Partial information about a system: represented by an operator ρ (the density matrix) which is: self-adjoint, non-negative, with $\operatorname{tr}\rho = 1$. In a basis it can be written as a convex combination of projectors:

$$\rho = \sum_i c_i \left|\phi_i\right\rangle \left\langle\phi_i\right|; \qquad \sum_i c_i = 1 \tag{1.1.14}$$

where the $\left|\phi_i\right\rangle$ are the possible states in which the sistem might be found, each with probability c_i. This definition comes from taking the expected value of a generic operator A given partial information on the system.

If we have a mixed state ρ, the expected value of an operator A is $\operatorname{Tr}(\rho A)$.

Representations A linear representation of a group is a map from it to the set of linear operators on a vector space, which preserves the group structure. The representation is *unitary* if the vector space is Hilbert, it is *projective* if it maps group elements to operator rays, and if the group has a topological structure it can be defined to be continuous wrt that topology.

We can also have representations of Lie algebras, defined analogously, and the following diagram commutes:

$$\begin{array}{ccc} G & \xrightarrow{T_e} & \mathrm{Lie}G \\ {\scriptstyle\mathcal{D}}\downarrow & & \downarrow{\scriptstyle\mathcal{D}} \\ \mathcal{L}(V) & \xrightarrow{T_e} & \mathcal{L}(V) \end{array}$$

Note that $\mathcal{L}(V)$ is just a fancy way of saying "operators on the Hilbert space", in our case.

Lie group It is a differentiable C^ω manifold with a group structure. We will treat *matrix* Lie groups.

We denote the coordinates on the group G as x, and the homeomorphisms of the atlas are denoted as $U(x) : \Omega \to G$, $\Omega \mathring{\subseteq} \mathbb{R}$.

Lie Algebra It is the tangent space to the identity of the Lie group G: T_eG. It is denoted as Lie$G$. From now on we speak of matrix Lie algebras.

It is endowed with a product, $[\cdot,\cdot]$, which corresponds to the commutator $[A,B] = AB - BA$, and so has its algebraic properties (bilinearity, antisymmetry, Jacobi, Leibniz). All the elements in a neighbourhood of $\mathbb{1}$ in the Lie group can be written as

$$U(x) = \exp\left(\sum_\alpha x_\alpha e_\alpha\right) \tag{1.1.15}$$

Its *structure constants* are defined by $[e_i, e_j] = f_{ij}^k e_k$.

Universal covering group Given a Lie group G, its universal covering $\tilde{G}$ is the (unique up to homeomorphisms) group which:

1. is homomorphic to G;
2. is simply connected;
3. has an isomorphic Lie algebra (Lie$G \simeq$ Lie$\tilde{G}$).

Experimental measurement A measurement is said to be of the first kind if by measuring again an sufficiently short time later the probability to find the same result gets arbitrarily close to 1. Otherwise, it is said to be of the second kind. First kind measurements obey the Von Neumann projection postulate.

Parity $\wp\psi(x) = \psi(-x)$. Its basic properties are $\wp^2 = \mathbb{1}$, $(1 \pm \wp)/2$ are projectors onto the subspaces of even/odd functions, if $\wp V = V$ then $[\wp, H] = 0$.

Compatibility Two observables $A_{1,2}$ are said to be compatible if, when the system is in an eigenstate for A_i, taking a type 1 measurement of A_{i+1} does not change the eigenvalue for A_i (but it can change the specific eigenvector in the eigenspace).

Families of observables For a set of observables $\mathcal{C} \ni A_i$, we say:

- the A_i are *independent* if $\nexists f$ such that $A_i = f(A_j)$, $i \neq j$;
- $\mathcal{C}$ is *complete* if it is a set of independent observables, maximal wrt inclusion;
- $\mathcal{C}$ is *irreducible* if any observable which commutes with all the observables in $\mathcal{C}$ is (a multiple of) the identity.

Tensor product If we have two Hilbert spaces $\mathcal{H}_{1,2}$, then their tensor product $\mathcal{H}_1 \otimes \mathcal{H}_2$ is the set of bilinear maps (improperly denoted as) $\phi \in (\mathcal{H}_1 \times \mathcal{H}_2)^{**}$, completed wrt the induced norm:

$$\Big(\langle\phi_1| \otimes \langle\phi_2|\Big)\Big(|\psi_1\rangle \otimes |\psi_2\rangle\Big) = \langle\phi_1|\psi_1\rangle \langle\phi_2|\psi_2\rangle \tag{1.1.16}$$

Also, we must take a quotient wrt having the same results when applied to couples of vectors.

So: not all tensors in $\mathcal{H}_1 \otimes \mathcal{H}_2$ are in the form $\phi_1 \otimes \phi_2$, but they all can be obtained by adding (finitely or infintely many) tensors expressed in this manner.

$$\forall \phi \in \mathcal{H}_1 \otimes \mathcal{H}_2 : \phi = \sum_{m,n=0}^{\infty} c_{mn} (\phi_m^1 \otimes \phi_n^2) \tag{1.1.17}$$

with ϕ_n^i belonging to $\mathcal{H}_i$ $\forall n$.

Product of operators It acts on the product of spaces, component by component, and we extend this definition by linearity and completeness. Again, not every operator on the tensor product can be written as the product of two operators in the spaces.

Symmetries A symmetry is a function from the algebra of observables into itself which preserves every expected value. Wavefunctions correspond to operators (dyads), which means a symmetry must preserve every transition probability, so Wigner's theorem applies. Symmetries which are continuous (ie have a group structure isomorphic to $\mathbb{R}$) cannot be represented by antiunitary operators.

Symmetries which preserve the Hamiltonian are said to be *dynamical*: they can be shown to be the ones which commute with the Hamiltonian.

Angular momentum A general angular momentum in $\mathbb{R}^3$ is a set of three functions with the algebra $[J_i, J_j] = i\hbar\varepsilon_{ijk} J_k$.

A particular case of this is the *orbital* angular momentum, $L_i = \varepsilon_{ijk} x_j p_k$.

Philosophical principles

- *Reality*: the world exists, and looks like our mathematical representation of it, whether or not we are measuring it;
- *Locality*: the evolution of a subsystem cannot be influenced by another subsystem if the spacetime interval separating them is spacelike;
- *Completeness*: the wavefunction contains all the information about a quantum system.

1.2 Axioms

States Pure states are represented by a ket $|\psi\rangle$ belonging to an abstract separable complex Hilbert space $\mathcal{H}$, modulo multiplication by a complex number. On $\mathcal{H}$ we have a scalar product $\langle \cdot | \cdot \rangle$, which is Hermitian. We furthermore assume the Fourier transform exists on $\mathcal{H}$.

Observables They are self-adjoint linear operators on $\mathcal{H}$, denoted as $\hat{A}$. Their norm is $\|A\| = \sup_{\|\psi\|=1} \|A\psi\|$. Their domain is denoted as $D(A)$.

The probability for a measure of A to be $\leq \lambda$ in a state ψ, with $\|\psi\| = 1$, is given by

$$P_\psi^A(\lambda) = \left| \langle \psi | P^A(\lambda) | \psi \rangle \right|^2 \tag{1.2.1}$$

Expectation value Denoted as $\langle \hat{A} \rangle_\psi$, it is calculated with: $\langle \psi | \hat{A} | \psi \rangle$. This is invariant wrt $\psi \to \alpha\psi$, $\alpha \in \mathbb{C}_0$; and assumes $\|\psi\| = 1$, otherwhise we should normalize dividing by its square norm.

Time evolution The postulate is that the transition probabilities between states are constant in time, and that time translation operators form a group isomorphic to $(\mathbb{R}, +)$. These two hypotheses imply that the time translation operator must be unitary.

Also, as in classical mechanics, the Hamiltonian generates time translations. So the time evolution operator is

$$U(t) = \exp\left(\frac{t\hat{H}}{i\hbar}\right) \tag{1.2.2}$$

To evolve a state which is not an eigenstate of the Hamiltonian we have to expand it in H's eigenbasis, where the H in the exponential in (1.2.2) becomes the single eigenstate's energy. Then $|\varepsilon\rangle$ evolves like

$$\exp\left(\frac{t\varepsilon}{i\hbar}\right) |\varepsilon\rangle \tag{1.2.3}$$

Von Neumann projection A first-kind measurement projects the state onto the eigenspace corresponding to the measured eigenvalue(s): if the result of the measuremnt is $\in \Delta$, the state of the system *instantaneously* changes to:

$$P^A_\Delta |\psi\rangle = \int \chi_\Delta(\lambda)\, \mathrm{d}P^A(\lambda)\, |\psi\rangle \tag{1.2.4}$$

where

$$\int_\Delta \mathrm{d}P^A(\lambda) = \frac{\mathbb{1}_\Delta}{\langle \psi | P^A(\Delta) | \psi \rangle} \tag{1.2.5}$$

(by $\mathbb{1}_\Delta$ we mean the projector onto the span of the eigenvectors corresponding to the eigenvalues $\lambda \in \Delta$: concretely, the formula is the same as (1.3.4) but the integral and summation are to be performed only over the $\lambda \in \Delta \cap \sigma(A)$.

1.3 Theorems

Riesz-Markov Let f be a positive linear functional defined from positive functions in the set C_0 (C^0 functions which go to 0 at $\pm\infty$) to $\mathbb{R}$. Then there exist a monotonically increasing function g such that, $\forall \psi \in C_0$:

$$f(\psi) = \int \psi(x)\, \mathrm{d}g(x) \tag{1.3.1}$$

Spectral families Spectral families are in bijection with self-adjoint operators. Finding the spectral family of an operator just means diagonalizing it; the operator A corresponding to the spectral familiy $P(\lambda)$ is given by its average over any state:

$$\langle \psi | A | \psi \rangle = \int \lambda\, \mathrm{d} \langle \psi | P(\lambda) | \psi \rangle \tag{1.3.2}$$

and the corresponding domain is

$$D(A) = \left\{ \psi \in \mathcal{H} : \int \lambda^2 \, \mathrm{d} \left\langle \psi \middle| P(\lambda) \middle| \psi \right\rangle < \infty \right\} \tag{1.3.3}$$

Completeness Given a self-adjoint operator A, we can always write the corresponding completeness with projectors corresponding to its eigenvectors. We have to account for the degeneracy: we can have a $d(\lambda)$-dimensional eigenspace corresponding to a single eigenvalue.

$$\mathbb{1} = \sum_{\lambda_n \in \sigma_d(A)} \sum_{r=1}^{d(\lambda_n)} |\lambda_n, r\rangle\langle\lambda_n, r| + \int_{\lambda \in \sigma_c(A)} \sum_{r=1}^{d(\lambda_n)} |\lambda, r\rangle\langle\lambda, r| \tag{1.3.4}$$

Wigner A map $\mathcal{H} \to \mathcal{H}$ which preserves the transition probabilities between states is represented by either a linear unitary operator ray $\hat{U} = \left\{ e^{i\alpha} U, \alpha \in \mathbb{R} \right\}$ or an antilinear operator ray $\hat{W} = \left\{ e^{i\alpha} W, \alpha \in \mathbb{R} \right\}$.

For linear operators we have $\left\langle U\phi \middle| U\psi \right\rangle = \left\langle \phi \middle| \psi \right\rangle$; for antilinear operators instead $\left\langle W\phi \middle| W\psi \right\rangle = \left\langle \phi \middle| \psi \right\rangle^*$.

Bargman There is a bijection between unitary continuous projective representations on G and unitary representations on its covering $\tilde{G}$.

Stone There is a bijection between one-parameter unitary transformation groups and self-adjoint operators: if we are given the transformation group $U(t)$ then we define

$$A = \frac{1}{i\hbar} \left. \frac{\mathrm{d}U}{\mathrm{d}t} \right|_{t=0} \in T_{\mathbb{1}}(G) \tag{1.3.5}$$

where the derivative is to be taken in a matrix sense, component by component. The constant i is necessary, the constant $\hbar$ is included for dimensional consistency. Then this A is self-adjoint in a dense domain $D(A)$.

On the other hand, if we are given a self-adjoint operator A we can exponentiate it into a one-parameter group of transformations:

$$U(t) = \exp\left(\frac{At}{i\hbar} \right) \tag{1.3.6}$$

Uncertainty principle We take two observables A and B, with domains such that, if we take the sets $D \subseteq D(A) \cap D(B)$ which are closed under application of both A and B, we can find a D which is dense in $\mathcal{H}$.

Then, recalling the definition of fluctuations in (1.1.8), we can state the theorem:

$$\Delta A_\psi \Delta B_\psi \geq \left| \frac{\left\langle \psi \middle| [A, B] \middle| \psi \right\rangle}{2i} \right| \tag{1.3.7}$$

This can be shown to also hold if instead of a pure state ψ we take our expectation values wrt a mixed state ρ.

The proof starts by considering the fact that the norm of

$$\left(\frac{\bar{A}}{\Delta A} \pm i \frac{\bar{B}}{\Delta B} \right) |\psi\rangle$$

(where $\bar{A} = A - \langle\psi|A|\psi\rangle$ and analogously for B) must be real and positive.

Compatibility For any two observables A, B: $[A,B] = 0 \iff$ they are compatible. (We proved it only in the case of bounded operators).

Also, $[A,B] = 0 \iff$ their spectral families commute.

Also, if $A = f(B)$ then $[A,B] = 0$ (and $\sigma \circ f = f \circ \sigma$ when applied to B).

Common eigenbasis A set of independent observables, having only discrete spectrum, is complete iff it has a set of common nondegenerate eigenvectors spanning the entire space $\mathcal{H}$.

If we denote $\vec{a}$ (with components a_i as the vector of the eigenvalues, that is, $A_i |\vec{a}\rangle = a_i |\vec{a}\rangle$, then we can write a completeness relation for the CSCO:

$$\mathbb{1} = \prod_{i=1}^{n} \left(\sum_{a_i \in \sigma_d} + \int_{a_i \in \sigma_c} \mathrm{d}a_i \right) |\vec{a}\rangle\langle\vec{a}| \tag{1.3.8}$$

Kato-Rellich Take a two-particle sysyem with a potential depending on their distance r, if: $U(r) \sim r^{-\alpha}$ near $r = 0$ with $a < 3/2$; $U(r) \sim 0$ near $r = \infty$, and $U(r) \in L^2([0,1], r^2\,\mathrm{d}r)$.

Then the domain of the Hamiltonian for each of the particles is the same as in the free particle case ($\psi \in L^2$ for the position, $p^2\tilde{\psi} \in L^2$ for the momentum).

Bloch If we have $H = p^2/(2m) + V(x)$ and V is periodic, such that $\exists a : \forall x : V(x+a) = V(x)$. Then the solution of the Schrödinger equation looks like

$$\psi(x) = U_k(x) e^{ik\cdot x} \tag{1.3.9}$$

With U_k being a periodic function (still with period a), and $|k| \leq \pi/a$ being the Bloch vector.

Perturbation theory If our Hamiltonian looks like $H = H_0 + V$, where V is a small[1] perturbation, we can write it as $H = H_0 + \lambda V$. We can also add more perturbation orders.

Then: we call the unperturbed eigenvalues ε_n^0, the perturbed eigenvalues up to order k ε_n^k. We normalize the eigenkets by choosing $\left\langle \varepsilon_n \middle| \varepsilon_n^0 \right\rangle = 1$, which means $\left\langle \varepsilon_n^k \middle| \varepsilon_n^0 \right\rangle = 0$ for $k \geq 1$.

We find the following closed formula for the eigenvalues: $\varepsilon_n^k = \left\langle \varepsilon_n^0 \middle| V \middle| \varepsilon_n^{k-1} \right\rangle$. For their eigenvectors, we find the components wrt the unperturbed eigenbasis by using an unperturbed completeness: $\left|\varepsilon_n^k\right\rangle = \sum_{n\neq m} \left|\varepsilon_m^0\right\rangle \left\langle \varepsilon_m^0 \middle| \varepsilon_n^k \right\rangle$, (the term with $n = m$ would be zero!) These components are:

$$\left\langle \varepsilon_m^0 \middle| \varepsilon_n^k \right\rangle = \frac{1}{\varepsilon_n^0 - \varepsilon_m^0} \left(\left\langle \varepsilon_m^0 \middle| V \middle| \varepsilon_n^{k-1} \right\rangle - \sum_{l=1}^{k} \varepsilon_m^l \left\langle \varepsilon_m^0 \middle| \varepsilon_n^{k-l} \right\rangle \right) \tag{1.3.10}$$

If we have degeneracy, that is, for a single eigenenergy there are many eigenvectors indexed as $|\varepsilon_{m,\alpha}\rangle$, we might be dividing by zero! but we can diagonalize the potential in the eigenspaces, so that $\left\langle \varepsilon_{m,\alpha}^0 \middle| V \middle| \varepsilon_{m,\beta}^0 \right\rangle = 0$ for $\alpha \neq \beta$. Then we can sum over the degeneracy as well, and we will not have any division by zero on a non-vanishing term.

[1] Note that we do not look at the absolute value of V but at the size of its effect.

1.4 Lemmas and observations

Probability function For any set $\Delta \in \mathcal{B}(\mathbb{R})$:

$$P_\Sigma^A(\Delta) = \langle \chi_\Delta \rangle_\Sigma \tag{1.4.1}$$

then:

$$P_\Sigma^A(]-\infty, \lambda]) = \langle \Theta(\lambda - A) \rangle_\Sigma \tag{1.4.2}$$

Symmetric operators Their expectation values $\langle \psi | A | \psi \rangle$ are real $\forall \psi \in D(A)$.

For a symmetric operator A, $\Delta A_\psi = 0 \implies A\psi = a\psi$, with $a = \langle A \rangle_\psi$.

The eigenstates of a symmetric are orthogonal: $\lambda_n \neq \lambda_m$ implies $\langle \lambda_n | \lambda_m \rangle = 0$.

Spectral theorem: we can find an orthonormal basis for $\mathcal{H}$ made of eigenstates of A. In this basis,

$$\langle A \rangle_\psi = \sum_n \lambda_n \frac{\left| \langle \lambda_n | \psi \rangle \right|^2}{\|\psi\|^2} \tag{1.4.3}$$

where $\left| \langle \lambda_n | \psi \rangle \right|^2 / \|\psi\|^2$ is then the probability of getting the measurement λ_n from an observation of A. From $\{|\lambda_n\rangle\}$ being a basis, then, we get $\Delta A_\psi = 0 \iff A\psi = a\psi$.

Projector representation of operators If A is self-adjoint, we can write it as

$$A = \sum_n \lambda_n \, |\lambda_n\rangle\langle\lambda_n| \tag{1.4.4}$$

which allows us to take functions of it, which then only act on the eigenvalues. So, we can calculate

$$\langle A \rangle_\psi = \int \lambda \mathrm{d} \left\langle \psi \middle| P^A(\lambda) \psi \right\rangle = \int \lambda \mathrm{d} P_\psi^A(\lambda) \tag{1.4.5}$$

with

$$P^A(\lambda) = \sum_n \Theta(\lambda - \lambda_n) \, |\lambda_n\rangle\langle\lambda_n| \tag{1.4.6}$$

On self-adjointness If A, B are self-adjoint: $A + B$ also is, AB generally is not; but

$$\frac{[A, B]}{i\hbar} \tag{1.4.7}$$

is.

Domain of H If $H = p^2/2m + V(x)$, its domain is not dense in $\mathcal{H}$ in general. However if either V is limited, or it has spherical symmmetry in 3D, then the domain of H coincides with that of p^2:

$$D(p^2) = \left\{ \psi \in L^2 : p^2 \tilde{\psi}(p) \in L^2 \right\} \tag{1.4.8}$$

Invariance of spectrum The spectrum of an observable A does not depend on the concrete Hilbert space: $\sigma(A) = \sigma(U^\dagger A U)$, U being the unitary operator which gives the isometry between Hilbert spaces.

Norm of operators In general we have that

$$\|A\| = \sup_{\lambda_n \in \sigma(A)} |\lambda_n| \tag{1.4.9}$$

Note that this extremum may be infinite.

On residual spectrum Self-adjoint operators and unitary operators do not have residual spectrum.

Probability measure in diagonal form Its discrete-spectrum part and continuous-spectrum part are derived by differentiating the definition of an abstract probability measure:

$$\mathrm{d}P^A(\lambda)\Big|_{\sigma_p(A)} = \sum_{\lambda_n \in \sigma_p(A)} \delta(\lambda - \lambda_n) \sum_{r=1}^{d(\lambda_n)} |\lambda_n, r\rangle\langle\lambda_n, r| \,\mathrm{d}\lambda \tag{1.4.10}$$

$$\mathrm{d}P^A(\lambda)\Big|_{\sigma_c(A)} = \sum_{r=1}^{d(\lambda)} |\lambda, r\rangle\langle\lambda, r| \,\mathrm{d}\lambda \tag{1.4.11}$$

Note that the integral of $\mathrm{d}P^A(\lambda)$ is 1.

Heisenberg approach, and Poisson brackets Instead of evolving the wavefuction $\psi \to U(t)\psi$ we can evolve the operators $A \to U^\dagger A U = A^H(t)$. This is equivalent to the Schrödinger approach.

The Poisson brackets between averages of operators on a fixed state are equal to averages of Lie brackets between the operators (divided by a factor of $i\hbar$:

$$\Big\{ \langle\psi|A|\psi\rangle \,,\, \langle\psi|B|\psi\rangle \Big\} = \left\langle \psi \left| \frac{[A,B]}{i\hbar} \right| \psi \right\rangle \tag{1.4.12}$$

Probability current Given any solution ψ to the Schrödinger equation with $H = p^2/2m + V(x)$, we want to find the continuity equation for the probability density $|\psi|^2$. To do this, writing SE for the Schrödinger equation, we calculate $\psi^* \mathrm{SE} - \psi \mathrm{SE}^*$, which after the manipulation $(b\partial^2 b^* - b^*\partial^2 b) = \partial(b\partial b^* - b^*\partial b)$ yields:

$$\partial_{tt}|\psi|^2 + \frac{\hbar}{2mi}\partial_x\left(\psi^*\partial_x\psi - \psi\partial_x\psi^*\right) = 0 \tag{1.4.13}$$

If we generalize this to 3 dimensions, then the current $\mathbf{j}$ in $\partial_t|\psi|^2 + \nabla\cdot\mathbf{j} = 0$ is

$$\mathbf{j} = \frac{\hbar}{2mi}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right) \tag{1.4.14}$$

Tensor product basics We can obtain a basis for the product space as $|e_i\rangle \otimes \left|e_j\right\rangle$, $i, j \in \mathbb{N}$.

It is known that for $\mathcal{H}_d = L^2(\mathbb{R}^d, \mathrm{d}^d x)$:

$$\mathcal{H}_d \otimes \mathbb{C}^N \simeq \bigoplus_{j=1}^{N} \mathcal{H}_d \qquad \mathcal{H}_n \otimes \mathcal{H}_m \simeq \mathcal{H}_{m+n} \tag{1.4.15}$$

We also have $L^2(\mathbb{R}^3, \mathrm{d}^3 x) = L^2(\mathbb{R} \ni r, r^2\,\mathrm{d}r) \otimes L^2(S^2 \ni (\theta, \phi), \sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi)$

A matrix identity For operators A and B, the following holds:

$$e^{-A} B e^{A} = \sum_{n=0}^{\infty} \frac{1}{n!} L_A^n(B) \tag{1.4.16}$$

where $L_A(B) = [B, A]$ is the operator which takes the commutator with A.

Representation of translations Translations, $\langle x| \to \langle x - a|$, are represented with

$$U(a) = \exp(a \cdot \nabla) = \exp\left(-\frac{a \cdot p}{i\hbar}\right) \tag{1.4.17}$$

since $\mathbb{R}^n$ is simply connected: a projective unitary representation is the same as a regular unitary representation, and we find this formula by differentiating the translated autobra, applied to a generic test ket.

Representation of rotations It can be shown that

$$\exp\left(\frac{\varphi L_3}{i\hbar}\right) x \exp\left(-\frac{\varphi L_3}{i\hbar}\right) = R(\hat{u}_3, \varphi) x \tag{1.4.18}$$

where $R(\hat{u}_3, \varphi)x$ is a rotation of angle φ around the z axis (by using formula (1.4.16)).

A generic rotation $\exp\left(-\varphi(L \cdot n)/i\hbar\right)$ must equal the identity if $\varphi \in 2\pi\mathbb{N}$: but then $\sigma(L \cdot n) \subseteq \hbar\mathbb{Z}$.

The universal covering of $SO(3)$ is unitarily represented in $\mathcal{H}$. $SO(3)$ is isomorphic to S^3 with all of its antipodes identified, or equivalently to unit quaternions or matrices in $SU(2)$ (still, with antipodes identified).

A unitary representation of $SU(2)$ is then a projective unitary representation of $SO(3)$. The algebra of its generators is the same as that of the generators of regular rotations (by the definition of universal covering),

Properties of angular momentum Angular momentum always obeys $[J^2, J_i] = 0$.

For a generic angular momentum we define: $J_\pm = J_1 \pm i J_2$. Then $[J_3, J_\pm] = \hbar J_\pm$.

$$J^2 = J_\pm J_\mp \pm \hbar J_3 + J_3^2 \tag{1.4.19}$$

We can prove that, for a simultaneous eigenvalue of J^2, J_3: $|\lambda m\rangle$ (where $J^2 |\lambda m\rangle = \hbar^2 \lambda |\lambda m\rangle$ and $J_3 |\lambda m\rangle = \hbar m |\lambda m\rangle$):

- $\lambda = j(j+1)$, $j \in \mathbb{N}/2$;
- $|m| \leq j$;
- j and m are either both half-integer of both integers;

- $\sigma(J^2, J_3)$ is *discrete*.

$$J_\pm |\lambda m\rangle = \hbar\sqrt{j(j+1) - m(m\pm 1)}\, |\lambda, m\pm 1\rangle \tag{1.4.20}$$

Orbital momentum Orbital momentum obeys $[L_i, x_j] = i\hbar\varepsilon_{ijk}x_k$, and an identical formula for p instead of x.

In spherical coordinates on S^2, we have $L_3 = -i\hbar\frac{\partial}{\partial\varphi}$. We can express $L_\pm$ and L^2; then by applying L_- repeatedly to $|ll\rangle$ (which satisfies $(L_+ |ll\rangle = 0)$ we can find the eigenfunctions. These are the spherical harmonics $Y_l^m(\theta, \varphi)$. For even/odd values of l they are even/odd. They form an orthonormal basis of $L^2(S^2, \mathrm{d}\Omega)$.

If we fix the total angular momentum in a specific direction we cannot precisely measure the directional momentum $n \cdot L$ in two different directions since they do not commute. We find

$$\Delta(L\cdot n)_\psi \Delta(L\cdot m)_\psi \geq \frac{\hbar}{2}\left|\langle\psi|(n\wedge m)\cdot L|\psi\rangle\right| \tag{1.4.21}$$

Spin A unitary representation of $SU(2)$ must be the one to generate spatial rotations. But the exponential of the orbital angular momentum is a representation of $SO(3)$: so there must be some other rotation. It cannot be something we simply add onto L as in $L + S$, still acting on $\mathbb{R}^3$, since then it would also not commute with position and momentum, but since those are irreducible it would necessarily be zero.

S must act on another space: so it must be that $\mathcal{H} = L^2(\mathbb{R}^3, \mathrm{d}^3x) \otimes \mathcal{H}_s$.

S will also be a rotation operator in $\mathcal{H}_s$, and since $\{x, p, S\}$ are an irreducible set of operators, and S^2 commutes with all of them, it must be constant. So a quantum particle is defined by its total spin $s \in \mathbb{N}/2$. S_3 can take all the values with integer difference from s, with absolute value less than or equal to it. Then we must have $\dim\mathcal{H}_s = 2s + 1$.

Using identity (1.4.15) we see that our system will be described by $2s + 1$ wavefunctions.

Spin 1/2 $\mathcal{H}_{1/2}$ is $\mathbb{C}^2$, so our operators are complex 2x2 matrices. The eigenvalues must be $\pm\hbar/2$, so we normalize by the absolute value of this and get $S = \frac{\hbar}{2}\sigma$, where σ is a 3-vector of 2x2 matrices. We can go to a basis in which one is diagonal: we take σ_3, then it will necessarily be $\left(\begin{smallmatrix}1 & 0\\ 0 & -1\end{smallmatrix}\right)$.

We now want to find σ_i for $i = 1, 2$. Since $\sigma_3^2 = \mathbb{1}$, it must be the same for the others. Also, they must be self-adjoint.[2]

We find the other two matrices, $\left(\begin{smallmatrix}0 & 1\\ 1 & 0\end{smallmatrix}\right)$ and $\left(\begin{smallmatrix}0 & -i\\ i & 0\end{smallmatrix}\right)$. We generally work in this basis, $|\uparrow\rangle_3$ and $|\downarrow\rangle_3$. The eigenvalues of $\sigma \cdot n$ for a generic unit vector $n \in S^2$ with the usual coordinates are:

$$\begin{pmatrix}|\uparrow\rangle_n\\ |\downarrow\rangle_n\end{pmatrix} = \begin{pmatrix}\cos(\theta/2)e^{-i\varphi/2} & \sin(\theta/2)e^{i\varphi/2}\\ -\sin(\theta/2)e^{-i\varphi/2} & \cos(\theta/2)e^{i\varphi/2}\end{pmatrix}\begin{pmatrix}|\uparrow\rangle_3\\ |\downarrow\rangle_3\end{pmatrix} \tag{1.4.22}$$

[2] We start by manipulating $0 = \sigma_z^2\sigma_y - \sigma_y\sigma_z^2$, then define the anticommutator...

Composition of angular momenta We have two angular momenta j_1, j_2. Their square and value along z can be simultaneously diagonalized; but we can also diagonalize their sum J^2 and J_z, along with j_1^2 and j_2^2.

We always keep the same eigenvalue for j_1^2 and j_2^2, and switch between the bases $|m_1\rangle\,|m_2\rangle$ and $|JM\rangle$. The combinations of m_1, m_2 corresponding to a single M is said to be a descending multiplet (in which J varies). We have the following isomorphism of Hilbert spaces:

$$\mathcal{H}_{j_1} \otimes \mathcal{H}_{j_2} = \bigoplus_{J=|j_1-j_2|}^{j_1+j_2} \mathcal{H}_J \tag{1.4.23}$$

where $\mathcal{H}_{j_i}$ are the spaces in which j_i has a fixed value, so they have an eigenbasis written as $\left|m_j\right\rangle$ (and analogously in $\mathcal{H}_J$ a basis is $|M\rangle$).

The spaces in (1.4.23) are those within which we work when treating a single particle (whose spin and orbital momentum do not change), but if we want to consider the general Hilbert space and write its completeness relation, we just take the direct sum of (1.4.23) for all possible values of j_1, j_2.

Clebsch-Gordan The coefficients which allow us to switch between the two bases are the *Clebsch-Gordan coefficients*: they are $(\langle j_1, m_1| \otimes \langle j_2, m_2|)\,|J, M\rangle$ (and we will denote $\langle j_1, m_1| \otimes \langle j_2, m_2|$ as $\langle j_1, m_1, j_2, m_2|$). In general they could be complex numbers, and to perform the inverse switch of basis we would have to take the conjugate: this is unwieldy, so (since we work in Hilbert spaces modulo a complex phase) we can take them to be real and positive.

They can be found in tables, but the way to calculate them if lost on an island filled with angry fermions is to start from $\langle j_1, m_1 = j_1, j_2, m_2 = j_2|J, M = J\rangle$ (both momentums are aligned), we can then repeatedly apply the operator $J_- = j_-^1 \otimes \mathbb{1} + \mathbb{1} \otimes j_-^2$ and calculate the eigenvalues with formula (1.4.20).

1.5 Specific problems

Wavepackets and constant potentials If our Hamiltonian is of the form $H = p^2/2m + V_0$ (we work in $\mathbb{R}$ for simplicity, but the generalizations to n dimensions are straightforward), its general eigenfunction ϕ_ε such that $H\phi_\varepsilon = \varepsilon\phi_\varepsilon$ is of the form

$$\phi_\varepsilon(x) = c_1 e^{ikx} + c_2 e^{-ikx} \tag{1.5.1}$$

with $k = \sqrt{2m(\varepsilon - V_0)}/\hbar$. Since k and ε are dependent on each other, we can write ϕ_k as well as ϕ_ε.

We can construct a packet of these eigenfunctions so that our wavefunction will be in $L^2(\mathbb{R})$:

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int_0^\infty f_{k_0}(k)\phi_k(x) \tag{1.5.2}$$

where $f_{k_0}(k)$ is a positive function with integral 1 and with a maximum in k_0.

If the potential V_0 is only locally constant, we can do this for every interval, and then connect the solutions by assuming continuity of the wavefunction and its first derivative.

General 1D potentials, qualitatively We take the usual Hamiltonian $H = p^2/2m + V(x)$, with $V(x)$ having finite limits at $\pm\infty$.

WLOG, we take the zero of the energy to be $\lim_{x\to+\infty} V(x)$, and also WLOG $\lim_{x\to-\infty} V(x) = V_\infty > 0$.

Then we have three cases. We write ε for the energy of the wavefunction. ε must be greater than the minimum value of the potential.

- $\varepsilon < 0$: we have discrete spectrum with degeneracy one;
- $0 < \varepsilon < V_\infty$: we have continuous spectrum with degeneracy one;
- $0 < V_\infty < \varepsilon$: we have continuous spectrum with degeneracy two.

Harmonic oscillator We start with a Hamiltonian $H = p^2/2m + m\omega^2x^2/2 = \hbar\omega(P^2 + X^2)/2$, with $X = x\sqrt{m\omega/\hbar}$, $P = p/\sqrt{m\omega\hbar}$. Note that it is a sum of squares, so the total energy must be positive.

We define $a = (X + iP)/\sqrt{2}$. Then we can see that $H = \hbar\omega(a^\dagger a + 1/2) = \hbar\omega H'$. So the spectrum of H' is just that of $a^\dagger a \equiv N$ plus a constant $1/2$.

We then find the algebra of these operators: $[a, a^\dagger] = 1$, $[a, N] = a$, $[N, a^\dagger] = a$ (note the inversion of the order in the commutators!).

By using the relation $Na = [N, a] + aN$ we can see that, if $N\psi = \lambda\psi$, $Na\psi = (\lambda - 1)\psi$, and analogously $Na^\dagger\psi = (\lambda + 1)\psi$. This means that if λ is an eigenvalue of N, $\lambda + m$, $m \in \mathbb{Z}$ also is.

However, λ must be nonnegative, since $\langle\psi|a^\dagger a|\psi\rangle \geq 0$. Therefore, $\forall\lambda : \exists m \in \mathbb{N} : a^m |\lambda\rangle = (\lambda - m)|\lambda\rangle = 0$. So the λ are actually just the natural numbers: this means that we can find all the eigenfunctions like $|n\rangle = (a^\dagger)^n |0\rangle$.

We just need to explicitly find $|0\rangle$, which satisfies $a|0\rangle = 0$. Since $p = -i\hbar\frac{\partial}{\partial x}$, we can see that $P = -i\frac{\partial}{\partial X}$. Therefore $a = X + \frac{\partial}{\partial X}$, and the solution to $a\psi = 0$ is a gaussian:

$$\langle X|0\rangle \propto \exp\left(-\frac{X^2}{2}\right) \tag{1.5.3}$$

Two-particle systems and Keplero We treat a two-particle system, in which they have a central potential $U(r)$ between them. By Kato-Rellich we do not have concerns about the domain of the Hamiltonian. We switch to center of mass (R) and vector distance (x) coordinates. We factor $\psi(R, x) = \varphi(R)\psi(x)$. This wavefunction satisfies the stationary Schrödinger equation, with the reduced masses appropriately adjusted (sum of masses and harmonic sum of masses).

The center-of-mass part is just a single particle Hamiltonian, which we know how to treat.

Since the Hamiltonian is rotationally invariant, our CSCO is $\left\{H, L^2, L_3\right\}$. We can split our Hilbert space into $L^2(R^+, r^2\,\mathrm{d}r)$ and $L^2(S^2, \mathrm{d}\Omega)$, in the first of which the CSCO is $\left\{H, L^2\right\}$ (quantum numbers ε, l); in the second of which the CSCO is $\left\{L^2, L_3\right\}$ (quantum numbers l, m).

By direct computation, the following holds:

$$P^2 = X^{-2}\Big(L^2 + (X\cdot P)^2 - i\hbar(X\cdot P)\Big) \tag{1.5.4}$$

We then write this in polar coordinates, and find that

$$P^2 = \frac{L^2}{r^2} - \hbar^2 \frac{1}{r}\frac{\partial^2}{\partial r^2} r \tag{1.5.5}$$

so our radial momentum is[3]

$$P_R = -i\hbar \frac{1}{r}\frac{\partial}{\partial r} r \tag{1.5.6}$$

The momentum in (1.5.6) can be shown to be self-adjoint in $L^2(\mathbb{R}^+, r^2\,\mathrm{d}r) \cap \{r\psi(\pm\infty) = 0\}$.

To simplify calculation we can go from the eigenfunctions $h_{\varepsilon l}$ to $\chi_{\varepsilon l} = r h_{\varepsilon l}$, which belong to $L^2(\mathbb{R}^+, \mathrm{d}r)$. This function obeys the equation:

$$-\hbar^2 \frac{\mathrm{d}^2}{\mathrm{d}r^2}\chi_{\varepsilon l} = \left(2m(\varepsilon - U(r)) - \frac{\hbar^2 l(l+1)}{r^2}\right)\chi_{\varepsilon l} \tag{1.5.7}$$

Which means that, just like the classical tractation of the problem, we can rewrite the equation to have an effective potential which includes the centrifugal barrier.

Spherical waves We treat the case of zero potential $U(r)$, which corresponds to free waves. We define $k = \sqrt{2m\varepsilon/\hbar^2}$. By plugging in a polynomial ansatz and imposing $\chi_{\varepsilon l}(0) = 0$ (which gives $h_{\varepsilon l} \sim r^l$, we find that $h_{kl}(r)$ (we write it with index k since there is a bijeciton between the ks and the εs) obeys

$$h_{kl}''' + \frac{2(l+1)h_{kl}''}{r} + \left(-\frac{2(l+1)}{r^2} + k^2\right)h_{kl}' = 0 \tag{1.5.8}$$

And we can check that $r h_{k(l+1)}$ obeys the same equation as h_{kl}'.

Also, for $l = 0$ we find the equation $\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} + k^2\right)\chi_{\varepsilon 0}$, which with the boundary condition gives us $\chi_{\varepsilon 0} \sim \sin(kr)$, so $h_{\varepsilon 0} \sim \sin(kr)/r$. These two facts together allow us to find the general $h_{\varepsilon l}$ (which we show with the right normalization):

$$h_{kl}(r) = \sqrt{\frac{2m}{k\pi}} k(-kr)^l \left(\frac{1}{kr}\frac{\mathrm{d}}{\mathrm{d}(kr)}\right)^l \frac{\sin(kr)}{kr} \tag{1.5.9}$$

These functions are not in L^2, so the spectrum of the Hamiltonian is continuous.

Coulomb potential We treat equation (1.5.7) with $U(r) = -e^2/r$, that is, a hydrogen atom. We define $a = \hbar^2/(mc^2)$, $\nu = 1/(ka)$, $x = 2kr$. The equation becomes:

$$\frac{\mathrm{d}^2\chi_{\varepsilon l}}{\mathrm{d}x^2} + \left(-\frac{1}{4} + \frac{\nu}{x} - \frac{l(l+1)}{x^2}\right)\chi_{\varepsilon l}(x) = 0 \tag{1.5.10}$$

We can construct an ansatz by requiring the solution to not diverge at 0 and ∞. This gives us $\chi_{\varepsilon l}(x) = x^{l+1}e^{-x/2}v_l(x)$, where $v_l(x)$ is an unknown function. We can expand it into a power series, $v_l(x) = \sum_p a_p x^p$. Throwing this into the equation gives us a recurrence formula:

$$a_{p+1} = -a_p \frac{\nu - l - 1 - p}{(p+1)p + (p+1)(2l+2)} \sim a_p/p \tag{1.5.11}$$

[3]Note that these are operators, so ∂r does not mean the derivative of r, but instead that when applied to a wavefunction ψ we need to calculate $\partial(r\psi)$.

This means that either the expansion for $v_l(x)$ terminates (ie it is a polynomial) or it is an exponential, $v_l(x) \sim e^x$, but this would mean that the whole solution diverges exponentially $\sim e^{x/2} \notin \mathcal{S}^*$. So it terminates: then we have a p_{max} for which the numerator in (1.5.11) is zero this means $\nu \in \mathbb{N}$, since all the other terms are!

By putting together the results we now have, we find the general form of the radial part of the solution of the Schrödinger equation for a Coulomb potential. It is written with Laguerre Polynomials:

$$L_j^k = \sum_{p=0}^{j} (-)^p \frac{(j-k)!}{(j-p)!(k+p)!j!} x^p \tag{1.5.12}$$

$$\chi_{nl}(x) = x^{l+1} e^{-x/2} L_{n-l-1}^{2l+1}\left(\frac{(2l+1)!(n-l-1)!}{(n+l)!}\right) \tag{1.5.13}$$

By differentiating the eigenfunction with the maximum angular momentum $l = n-1$, we can find the r for which the probability of finding the particle is largest, which is $r = n^2 a = n^2\hbar^2/(mc^2)$

Landau levels If we have a spinless quantum particle in a plane with a perpendicular magnetic field, the spectrum of the Hamiltonian is just like that of a harmonic oscillator, with $\omega = eB/m$.

Scattering We consider a particle impacting a target, and we impose the following conditions: the impact must be (relativistically) elastic; the distance between the scattering centers must be larger than their potentials' influence and the target is thin enough (so we can consider just one scattering center).

We want to calculate the differential scattering cross section $\sigma(\theta,\varphi) = \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}$, which is the ratio of the differential probability densities of being scattered in the solid angle $\mathrm{d}\Omega$ when coming from the differential area $\mathrm{d}\sigma$. If we know the impacting and diffused probability currents j_i and j_d, the differential scattering cross section is: $\sigma(\theta,\varphi) = r^2 \left|j_d \cdot r\right| / \left|j_i\right|$ (the formula is like this because we want this to be invariant wrt going further away from the scattering point: the current density will decrease like $1/r^2$, so we multiply by r^2).

If we treat the scattering as if it was stationary, and consider an asymptotic wavefunction:

$$\psi(x) = \exp\left(\frac{t\varepsilon}{i\hbar}\right)\left(\exp\left(-\frac{p\cdot x}{i\hbar}\right) + \frac{f_p(\theta,\varphi)}{r}\exp\left(-\frac{pr}{i\hbar}\right)\right) \tag{1.5.14}$$

If we calculate the diffused and incident currents (with the help of the probability conservation formula), we find that the scattering cross section to be $\sigma(\theta,\varphi) = \left|f_p(\theta,\varphi)\right|^2$.

This also holds for the generic case.

Nonstationary case We wish to solve $H\left|\psi\right\rangle = (H_0 + V)\left|\psi\right\rangle = E\left|\psi\right\rangle$, where H_0 is the free particle Hamiltonian, ie $-\hbar^2\nabla^2/(2m)$. We know that the Schrödinger equation must be satisfied everywhere, even at infinity where $V = 0$. So E is the energy corresponding just to H_0 (since it must be conserved). Now, we define $\Omega^{-1} = 1/(E - H_0 \pm i\varepsilon)$ as a formal operator which inverts $E - H_0$. Then, inserting a spatial completeness, and denoting ψ_{HOM} as the solution of the homogeneous equation ($(E - H_0)\psi_{HOM} = 0$), we have:

$$\langle x|\psi\rangle = \langle x|\psi_{HOM}\rangle + \int \mathrm{d}^3y \, \langle x| \, \Omega^{-1} \, |y\rangle\langle y| \, V \, |\psi\rangle \tag{1.5.15}$$

Note that $\langle y| \, V \, |\psi\rangle$ just means $V(y)\psi(y)$.

We can find the matrix elements $\langle x| \, \Omega^{-1} \, |y\rangle$ by inserting a momentum completeness (we denote the variable momentum as q, and the momentum eigenvalue corresponding to E as p):

$$\langle x| \, \Omega^{-1} \, |y\rangle = \int \mathrm{d}^3q \, \langle x| \, \Omega^{-1} \, |q\rangle\langle q| \, |y\rangle = \int \mathrm{d}^3q \, \frac{1}{(p^2 - q^2)/2m \pm i\varepsilon} \frac{e^{q\cdot(x-y)/(i\hbar)}}{\sqrt{2\pi}} \tag{1.5.16}$$

Now, we create a wavepacket with a small momentum uncertainty, such that the position uncertainty is much larger than the wavelength. Also, the position uncertainty must be larger than the width of the scattering cross section total ($\int \sigma \, \mathrm{d}\Omega$). Also, we do not consider any interference between incoming and diffused wavefunction.

So, we know how to solve the eigenvalue problem to find the incoming ψ_{in} — note that we have fixed E, the eigenvalue for the free Hamiltonian. Now, we can construct a wavepacket with some momentums around p_0, distributed according to $g_{p_0}(p)$ (which, without being too specific, should look like a symmetric and rather sharp peak around p_0). We also evolve each eigenfunction in this wavepacket.

$$\psi(x,t) = \int g_{p_0}(p) e^{\frac{\varepsilon t}{i\hbar}} \psi_{IN}(x) \mathrm{d}^3p \tag{1.5.17}$$

This looks like a small packet happily travelling along with speed p_0/m. We need to do a lot of calculations and approximations to solve this integral; and after doing so we find that the differential scattering cross section depends on a function of the incoming wave:

$$f_P(\theta,\varphi) = -\frac{2m}{k} \int \frac{\mathrm{d}^3y}{4\pi} V(y)\psi_{IN}(y) e^{-ipr\cdot y} \tag{1.5.18}$$

To actually calculate σ, we integrate the probability density of the outgoing wavefunction, multiplied by r^2, along an outgoing ray, and divide it by the integral of the probability density of the incoming function over a line parallel to the propagation direction. We then get $\sigma = |f_P|^2$.

Particle swaps We treat a many-particle system: it is described in $\mathcal{H}^{\otimes N}$. In this space we want to find a unitary representation of the operation of switching particles. The group of particle permutation $S_N \ni \sigma$ is generated by adjacent particle swaps σ_i, and it obeys the properties: $[\sigma_i\sigma_j] = 0$ when $|i-j| > 2$; $\sigma_i\sigma_{i+1}\sigma_i = \sigma_{i+1}\sigma_i\sigma_{i+1}$.

The representation of this group can be said tom just remap the basis vectors e_{ij} to $e_{i\sigma j}$.

In general, by the unitarity of the representation of a swap $U(\sigma)$, it needs to hold that $U(\sigma) \, |\psi\rangle = c \, |\psi\rangle$ for some $c \in \mathbb{C}$.

Superselection sectors *If* it holds that $\sigma_i^2 = \mathbb{1}$, then $c = \pm 1$. c must be the same for all particles in a set of identical particles we are allowed to swap (otherwise we would have a contradiction by the rule $\sigma_i\sigma_{i+1}\sigma_i = \sigma_{i+1}\sigma_i\sigma_{i+1}$). Then, we can distinguish *fermions* for which $c = -1$ and *bosons* for which $c = +1$. This immediately gives us the Pauli exclusion principle.

Fractionary quantum Hall effect If it is not the case that $\sigma_i^2 = \mathbb{1}$, then the orientation of the swaps matters, we need to keep track of it ($\sigma_i^+ \neq \sigma_i^-$). we must still have $U(\sigma)\left|\psi\right\rangle = c\left|\psi\right\rangle$, but now $c = e^{i\theta}$ for *any* theta. These are braid statistics The particles obeying these statistics are called anyons.

We can see this in an experiment. We create an almost two dimensional system, by having two charged semiconductor plates near each other with a magnetic field. We see Landau levels ($\sim$ harmonic oscillator energy levels), but because of impurities we also observe slight imperfections in the energy distribution. This is the whole Hall effect.

Now, at very low temperatures, our particles (e^-) are almost all the the lowest energy level ($n\hbar c/(eB) = 1/3$) and they obey braid statistics with $\theta = 2\pi/3$: their wavefunction is

$$\psi(z_1, \dots, z_n) = \prod_{i<j}(z_i - z_j)^{1/3} \prod_{i=1}^{N} e^{-i|B|^2} \tag{1.5.19}$$

Aharonov-Bohm We try to define a self-adjoint momentum operator on $\mathbb{R}/\sim$, where $x \sim x + 2\pi$. The condition to satisfy is $\phi^*(x)\psi(x)\big|_0^{2\pi} = 0$.

We find that $\phi(2\pi) = e^{i\gamma}\phi(0)$ is sufficient (although the naîve $\gamma = 0$ also works). We call this momentum P_γ. Its eigenfunctions look like $\exp\left(\frac{i\gamma}{2\pi}\right)\psi_n = A\psi_n$, where ψ_n is an eigenfunction of P_0.

Then, $P_\gamma = A^\dagger P_0 A$, therefore we can calculate: $P_0 + \frac{\gamma\hbar}{2\pi} = P_\gamma$.

This is physically realized by putting an infinite radially small solenoid through the ring on which the particle lives. We can then perform the canonical substitution $p \to p - eA/c$ with $-eA/c = \gamma\hbar/(2\pi)$. This implies an observable shift in the spectrum of the momentum, which is observable experimentally.

Berry phase The result which expresses this generally is that when going around a loop C the wavefunction gains a phase given by:

$$e^{i\gamma} = \exp\left(\oint_C \left\langle\psi|\mathrm{d}\psi\right\rangle\right) \tag{1.5.20}$$

EPR We can see experimentally that $\neg(R \wedge L \wedge C)$, and that also $\neg(R \wedge L \wedge \neg C)$.

We see this by having N spinless particles decaying into two fermions with spin $1/2$. Their state is thus $\left|\psi\right\rangle = (\left|\uparrow\right\rangle_A \left|\downarrow\right\rangle_B - \left|\downarrow\right\rangle_A \left|\uparrow\right\rangle_B)/\sqrt{2}$.

Now, we measure one of them and then see that the other always has the opposite spin. After the measurement, we see around $N/2$ of them with $\left|\uparrow\right\rangle_A \left|\downarrow\right\rangle_B$ and $N/2$ with $\left|\downarrow\right\rangle_A \left|\uparrow\right\rangle_B$.

So, were they in a mixed state before the measurement? No, since we can compute that the expected value for the spin in the x direction is 0 for the superposition, and $1/4$ for the mixed state.

Then, in the time interval between the moment when the supports of the particles start having spacelike distance, and when the measurement is done (on A), we have a contradiction: is B in a mixed state, or in a superposition? If $R + L + C$ were the case, both. Experiment says "superposition".

Bell inequalities We take a two-fermion system, with spins S_A and S_B, and define:

$$B(\{u_i\}_i) = S_A \cdot u_0 \otimes (S_B \cdot u_1 - S_B \cdot u_2) + S_A \cdot u_3 \otimes (S_B \cdot u_1 + S_B \cdot u_2) \tag{1.5.21}$$

where u_i are 4 unit vectors, and we define the angles θ_i, $i = 1, 2, 3, 4$ to be the ones between $(u\dots)$ 01, 02, 13, 32 respectively. Then $\theta_1 + \theta_3 + \theta_4 = \theta_2$.

If we take a classical approach to calculating B, by making it have a probability distribution wrt a parameter λ, we see that it must be $|B| \leq 1/2$.

If, instead, we compute $\langle\psi|B|\psi\rangle$ by allowing for superpositions, we get a different result. Call $|\pm\rangle_{A,B}$ the eigenvector corresponding to spin up/down along the z direction for particle A, B. Then, for both particles, we can calculate the following values for the spin a given unit vector $u(\theta, \varphi) \in S^2$:

$$\langle\pm|S \cdot u|\pm\rangle = \pm\frac{\cos\theta}{2} \qquad \langle\pm|\, S \cdot u\, |\mp\rangle = \frac{1}{2}\sin\theta e^{\pm i\varphi} \tag{1.5.22}$$

Note that the second term is crucial for the interference! Using this, we calculate

$$\langle\psi|(S_A \cdot u)(S_B \cdot u')|\psi\rangle = -\frac{\cos(\theta - \theta')}{4} \tag{1.5.23}$$

Now, we take $\theta_1 = \theta_3 = \theta_4 \equiv \theta$, so $\theta_2 = 3\theta$. So $\langle\psi|B|\psi\rangle = -(3\cos\theta - \cos(3\theta)/4$, which has a maximum in $\theta = \pi/4, 3\pi/4$. There, $\langle\psi|B|\psi\rangle = \pm 1/\sqrt{2}$. This is incompatible with $|B| \leq 1/2$.

Chapter 2

Nuclear physics

2.1 Introduction

Things to remember about nuclear units: $\hbar c \approx 197\,\text{MeVfm}$ and $\text{MeVfm} = 10\,\text{eVÅ}$; there are weird things like $e^2 = 1.44\,\text{MeVfm}$, $4\pi\varepsilon_0 = 1$. The atomic mass unit is equal to 931.5 MeV.

We have indetermination both between position and momentum: $\Delta x \Delta p \geq \hbar/2$ and between time and energy: $\Delta E \Delta t \geq \hbar/2$.

We can characterize the atomic particles by mass m, charge q, spin s, half-life and mean charge radius $\left\langle \rho r^2 \right\rangle \sqrt{c}$: this last quantity is of the order 0.87 fm for the proton, and -0.1 fm for the neutron.

2.2 Nuclear density

It it roughly constant up to some radius, then it decays. The proper way to write it would be to sum the modulus square of the wavefunction ψ_i of every nucleon:

$$\rho(r) = \sum_i \left|\psi_i(r)\right|^2 \tag{2.2.1}$$

We can approximate it as a radial distribution

$$\rho(r) \sim \frac{\rho_0}{1 + \exp\left(\frac{r - r_0}{a}\right)} \tag{2.2.2}$$

where $\rho_0 \approx 0.15 \div 0.2\,\text{nucleons/fm}^3$ is the approximately constant density in the central region, $r_0 \approx 1.20 \div 1.25\,\text{fm} A^{1/3}$ is the approximate radius of the nucleus (corresponding to where the density becomes half of ρ_0), $a \approx 0.65 \div 0.7$ fm is the *diffusivity*, which quantifies the length scale at which the density distribution goes to zero.

Taking $r_0 \approx 1.2$ fm, we can estimate the nucleon density

$$\rho_0 \approx \frac{A}{V} = \frac{A}{\frac{4}{3}\pi\left(r_0 A^{1/3}\right)^3} \approx 0.138\,\text{fm}^{-3} \tag{2.2.3}$$

and the corresponding mass density will be $\approx 129\,\text{MeV/fm}^3$ corresponding to $2.3 \times 10^{17}\,\text{kg/m}^3$, which is huge when compared to, say, that of a block of Osmium, which is around $2.26 \times 10^5\,\text{kg/m}^3$.

There are also asymmetric effects, such as a skin of neutrons in the outermost part of the nucleus or a halo, which extends much further than a skin. This can be seen by looking at the differences in the scattering cross section $\sigma \approx \pi r_0^2$.

We distinguish the nuclei by the proton number Z, the neutron number N and their sum $A = N + Z$. They are written as ${}^{A}[Z]$.

- Isotopes have the same Z, ^{235}U and ^{233}U;
- Isobares have the same A, ^{44}Ca and ^{44}Ti;
- Isotones have the same N, ^{40}Ca and ^{38}Ar;
- Isomeres have the same Z and N, but are in different excitation states. We require them to be somewhat stable, with half-life $\gtrsim 10^{-12}$ s, ^{99}Tc and ^{99m}Tc.

We also define specular nuclei: denoting the nuclear numbers as (N, Z), (a, b) is isobaric and specular to (b, a).

At the driplines, the excess nucleons are not bound (the effective potential they are in does not have a minimum).
^{8}B and ^{8}Be are isobares.
^{19}F is an isotone to ^{17}F.
The stable isotopes of Samarium are those with $A = 144, 150, 152, 154$.
The specular nuclide to ^{11}Li would be ^{11}O, but it does not seem to exist.

The mass of a nuclide is given by

$$M(A, Z) = Zm_p + (A - Z)m_n - B(A, Z) \tag{2.2.4}$$

where B is the binding energy. It is a good first approximation to say $B/A \approx$ const, around 8 MeV.

Actually, this value increases up to iron, then very slowly decreases, with slight bumps at magic numbers.

2.3 Waterdrop model

A nucleus is similar to a water droplet, like:

- $\nabla \cdot \vec{v} = 0$ and similarly the nucleons are roughly incompressible, mantaining a constant density inside the nucleus;
- The evaporation heat of a water drop is directly proportional to its mass, and similarly we can approximate $B \propto A$;
- The water molecules are held together by intermolecular Van der Waals forces, with expressions like $r^{-12} - r^{-6}$, and similarly the strong nuclear force has a short range.

We can write a Semi Empiric Mass Formula, which will give us the best estimate of the waterdrop model for the nuclear mass. We will assume that the nuclear forces *saturate* after a certain point, that is, they have finite support.

Volume term The full potential is

$$V = \sum_{i<j} V_{ij}(\left|r_i - r_j\right|) \tag{2.3.1}$$

so if the nuclear force was long-range we would have $B \propto A(A-1)\langle V\rangle$, since the terms in the sum (2.3.1) are $A(A-1)/2$ (by $\langle V\rangle$ I mean the average binding energy in a nucleon pair).

We must account for the fact that the nucleons only interact with their neighbours in some fixed volume V_{int}: so

$$B \propto \frac{A(A-1)V_{\text{int}}}{\underbrace{V_{\text{total}}}_{\propto A}} \propto A - 1 \sim A \tag{2.3.2}$$

So our first term will be

$$B \sim a_V A \tag{2.3.3}$$

Surface term The surface nucleons interact with less nucleons than the internal ones. This effect will surely be negative and proportional to the surface area, and we are only interested in proportionality, so

$$B \sim a_V A - a_S A^{2/3} \tag{2.3.4}$$

Coulomb term The positively charged nucleons repel each other: we model the nucleus as a uniformly charged sphere, which will have charge density $\rho = 3Ze/\left(4\pi R^3\right)$, where R is the radius of the nucleus. Applying $\nabla \cdot E = \rho/\varepsilon_0$ and integrating over a sphere of radius r, we get

$$E(r) = \begin{cases} \frac{Zer}{4\pi\varepsilon_0 R^3} = \frac{\rho r}{4\varepsilon_0} & r \leq R \\ \frac{Ze}{4\pi\varepsilon_0 r^2} = \frac{\rho R^3}{3\varepsilon r^2} & r \geq R \end{cases} \tag{2.3.5}$$

The energy density of the electric field is given by $u = \varepsilon_0 E^2/2$; its integral over all of space $U = 4\pi \int_0^\infty ur^2\,\mathrm{d}r$, which corresponds to the Coulomb term to subtract to the binding energy, can be calculated analytically, and is the sum of the external and internal contributions:

$$U = \left(1 + \frac{1}{5}\right)\frac{(Ze)^2}{8\pi\varepsilon R} \tag{2.3.6}$$

Then we can put all the constants into a term, leaving out only the proportionalities to Z^2 and $R^{-1} \propto A^{-1/3}$. Now our formula is:

$$B \sim a_V A - a_S A^{2/3} - a_C Z^2 A^{-1/3} \tag{2.3.7}$$

with

$$a_C = \frac{3}{5}\frac{e^2}{4\pi\varepsilon_0}\frac{1}{r_0} \approx 0.7\,\text{MeV} \tag{2.3.8}$$

which can be found by recalling $e^2 = e^2/(4\pi\varepsilon_0) \approx 1.44\,\text{MeVfm}$ and $r_0 \approx 1.2 \div 1.3\,\text{fm}$.

It might be more accurate for this term to be proportional to $Z(Z-1)$, since the proper expression for the energy will be:

$$U = \frac{e^2}{4\pi\varepsilon_0}\sum_{i=1}^{Z}\sum_{j<i}\frac{1}{\left|r_i - r_j\right|} \propto \frac{Z(Z-1)}{|\bar{r}|} \propto \frac{Z(Z-1)}{A^{1/3}} \tag{2.3.9}$$

where $\bar{r}$ is the average distance between the protons in the nucleus. We do not know what it looks like, but surely $\bar{r} \propto r_{\text{nucleus}} \propto A^{1/3}$.

Asymmetry term The binding energy between pp is similar to that between nn, let us call it v, but it is smaller than the pn attraction by a factor ~ 2, so let us call the np energy $2v$. This can be seen empirically from the fact that nn and pp are not bound states, while the deuton (^{2}H) is. The factor is around 2 because of the Pauli exclusion principle: nucleons are spin$-1/2$ fermions, so if their spins and isospins are the same they cannot come near one another: the spins will be aligned around half of the times that the isospins are aligned, so this justifies the factor of 2.

The asymmetry term becomes relevant for large A.

When counting the total binding energy we must divide by A to account for the fact that every nucleon only interacts with its neighbours.

$$\begin{aligned} B_A &= \frac{Nv}{A}(N+2P) + \frac{Pv}{A}(2N+P) && \text{(2.3.10a)}\\ &= \frac{v}{A}\Big(N^2+P^2+4NP\Big) && \text{(2.3.10b)}\\ &= \frac{v}{2A}\Big(3N^2+3P^2+6NP-N^2-P^2+2NP\Big) && \text{(2.3.10c)}\\ &= \frac{v}{2A}\Big(3A^2-(N-Z)^2\Big) && \text{(2.3.10d)} \end{aligned}$$

The linear term in A is the volumetric term; the term to add is $\propto (N-Z)^2/A$. So now we have

$$B \sim a_V A - a_S A^{2/3} - a_C Z^2 A^{-1/3} - a_A \frac{(N-Z)^2}{A} \tag{2.3.11}$$

This can be also seen by approximating the nucleus as a Fermi sea: if $N = Z$ all the nucleons can be at the Fermi energy ε_F, while if there is a difference some of them will have more energy.

Take $N - Z = 4i$, with $i \in \mathbb{N}$, and imagine moving to this configuration from $i = 0$. The first two protons becoming neutrons will raise the energy of the nucleus by $2\Delta E$, where ΔE is the separation between the energy levels. The next step will take $6\Delta E$, and in general the $j+1$-th will take $2(2j+1)\Delta E$: we need to add these up,

$$\sum_{j=1}^{i} 2(2j+1)\Delta E = 2i^2\Delta E = 2\frac{(N-Z)^2}{16}\Delta E \tag{2.3.12}$$

It can also be shown (CHECK LATER) that $\Delta E \propto 1/A$. Then we get the same formula as before.

Pairing term It is added to the formula to explain the experimental data: the term we need to add looks like

$$B_P = \frac{a_P}{A^{1/2}} \qquad a_P = \begin{cases} +\delta & \text{even-even} \\ 0 & \text{even-odd} \\ -\delta & \text{odd-odd} \end{cases} \tag{2.3.13}$$

with $\delta \sim 11 \div 12\,\text{MeV}$. It is due to the wavefunctions of the nuclides "pairing up" in some sense. The exponent being $1/2$ is not certain, some say $3/4$ fits the data better...

SEMF The full formula looks like

$$B \sim a_V A - a_S A^{2/3} - a_C Z^2 A^{-1/3} - a_A \frac{(N-Z)^2}{A} \pm \frac{a_P}{A^{1/2}} \tag{2.3.14}$$

with $a_V \approx 16\,\text{MeV}$, $a_S \approx 17\,\text{MeV}$, $a_C \approx 0.7\,\text{MeV}$, $a_A \approx 23\,\text{MeV}$, $a_P \approx 12\,\text{MeV}$. It fits the data well, for $A > 10 \div 20$.

The empirical data do not exactly follow the SEMF: the binding energy is slightly higher at certain *magic numbers*.

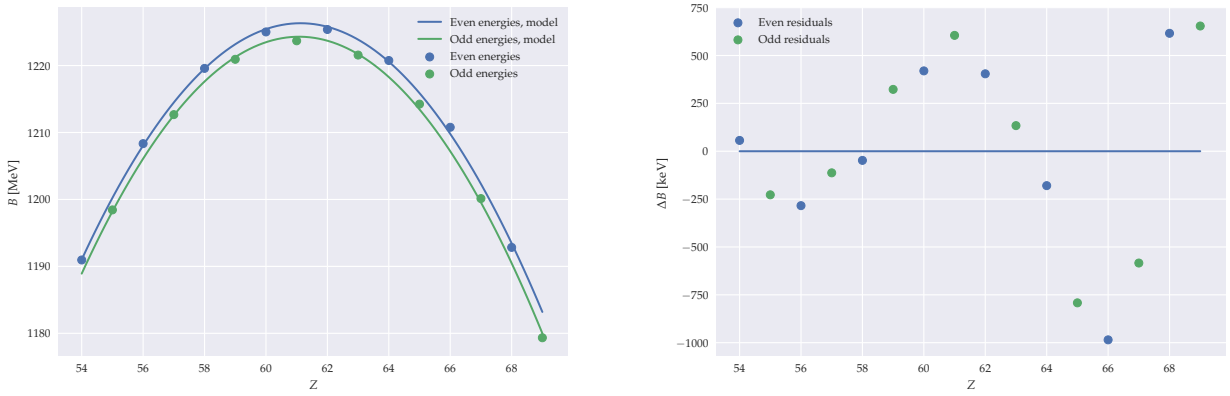
The highest binding energy per nucleon is found with ^{62}Ni ($B/A = 8.7945\,\text{MeV}$), while the lowest mass per nucleon is found with ^{56}Fe. They can be different because they have different proton/neutron ratios.

Mass parables If we work at fixed A, the (2.3.14) looks like a parabola wrt Z. Actually, if A is even it looks like two parabolas, distanced 2δ apart, with the nuclides switching from one to the other as the parity of Z changes; if A is odd the nuclides are always even-odd so it is just one parabola. The asymmetry term is proportional to $(A-2Z)^2$, so we get:

$$B = Z^2\left(-a_C A^{-1/3} - \frac{4a_A}{A}\right) + Z(4a_A) + \text{const} \tag{2.3.15}$$

We perform a parabolic fit for the nuclei at $A = 148$, and compute the coefficients corresponding to the fit parameters according to formula (2.3.15). The results are shown in 2.1.

The fit parameters give $a_A = 21.41\,\text{MeV}$, $a_C = 0.65\,\text{MeV}$, $a_P = 12.26\,\text{MeV}$. The energy at the vertex of the parabola can be calculated from the model assuming $a_V = 16\,\text{MeV}$ and $a_S = 17\,\text{MeV}$ to be 1340 MeV, while the real energy is 1225 MeV.



(a) Fit and raw data

(b) Residuals of the fit

Figure 2.1: Mass parabola fit

There are some odd-odd stable nuclei, like ^{14}N, but they are rare.

Specular nuclei If they have $\Delta Z = 1$ and A is odd, interesting things happen. Our working example is $^{15}_{8}O_7$ and $^{15}_{7}N_8$.

The only term which changes in the SEMF between them is the Coulomb term: their Zs are $(A \pm 1)/2$, therefore (applying the corrected Coulomb formula given in (2.3.9)) their difference in energy is given by

$$\Delta B = \frac{a_C}{A^{1/3}} \left(\frac{(A+1)(A-1)}{4} - \frac{(A-1)(A-3)}{4} \right) \tag{2.3.16a}$$

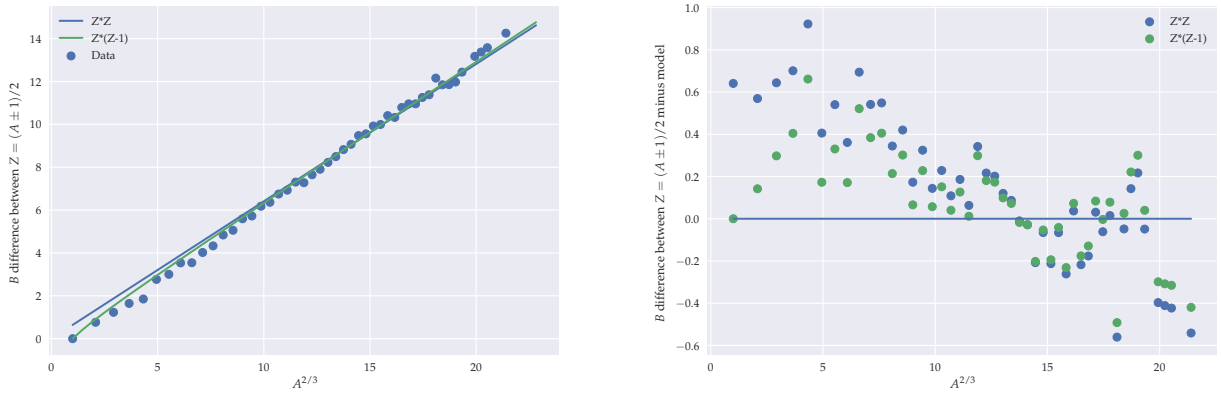
$$= \frac{a_C}{A^{1/3}} \left(\frac{4A-4}{4} \right) \tag{2.3.16b}$$

$$= a_C \left(A^{2/3} - A^{-1/3} \right) \tag{2.3.16c}$$

We can plot the data for ΔB wrt $x \overset{\text{def}}{=} A^{2/3}$. The plot will be of the form

$$\Delta B = a_C x - \frac{a_C}{\sqrt{x}} \tag{2.3.17}$$

The fit works, giving us $a_C = (631 \pm 5)$ keV in this parametrization.



(a) Fit

(b) Residuals

Figure 2.2: Fit of the difference in B between symmetric nuclei. The chi square is $0.136\,\mathrm{MeV}^2$ for the Z^2 model, and $0.062\,\mathrm{MeV}^2$ for the $Z(Z-1)$ model.

2.4 Fermi gas model

Hypotheses

- The nucleons are spin $1/2$ fermions;
- the nucleons' collective actions can be represented with a spherically symmetric potential well $U(r)$, extended in a radius $R = r_0 A^{1/3}$;
- the nucleon gas is degenerate: the kinetic energy of the nucleons is much less than the thermal energy $k_B T$.

The proper Hamiltonian, without the mean-field approximation, would be

$$H = \sum_i T_i + \sum_{i<j} V_{ij}\left(\left|r_i - r_j\right|\right) \tag{2.4.1}$$

instead, we use

$$H_{\mathrm{sp}} = -\frac{\hbar^2 \nabla^2}{2\mu} + U(r) \tag{2.4.2}$$

where sp means 'single particle', $\mu^{-1} = m_{\mathrm{sp}}^{-1} + m_{\mathrm{nucleus}}^{-1}$.

For nuclei at human temperatures, $\lesssim 10^3\,\mathrm{K}$, we have energies $\lesssim \frac{3}{2} k_B T = 0.13\,\mathrm{eV} \ll MeV$, so thermal motion is negligible.

$1D$ infinite well We have an infinite well from $-a/2$ to $a/2$, and inside it a particle of mass m.

The solutions to the time-independent Schrödinger equation are in the form

$$\psi(x) = A\sin(kx) + B\cos(kx) \tag{2.4.3}$$

where $k^2 = 2mE/\hbar^2$ is the square of the wavenumber, which is directly proportional to the momentum $k = p/\hbar = 2\pi/\lambda$. We must also consider the boundary conditions: the domain of the Hamiltonian is $\left\{\psi(x) \in L^2 \,|\, \psi(\pm a/2) = 0\right\}$.

So we have two classes of solutions, proportional to either $\cos\big((2q)\pi x/a\big)$ or $\sin\big((2q+1)\pi x/a\big)$ with $n \in \mathbb{N}$. If we call the even or odd number $2q(+1) = n_x$, the energy comes out to be

$$E = \frac{\hbar^2 k^2}{2m} = \frac{h^2 n_x^2}{8ma^2} \tag{2.4.4}$$

$3D$ **potential well** The problem works out analogously, with

$$E = \frac{h^2}{8ma^2} \sum_i n_i^2 \tag{2.4.5}$$

so we work in the space $\mathbb{Z}_+^3 \ni \vec{n}$, where same-energy states live in spherical shells.

The differential number of states in these shells is (approximately) given by the volume of the shell, which is an eighth of the sphere's: $N = \frac{1}{8} 4\pi n^2 \,\mathrm{d}n$. This can also be written as $\rho(E)\,\mathrm{d}E$, that is, it corresponds to a density of states.

Then, since the energy is just a function of n, we have

$$\mathrm{d}E = \frac{h^2}{8ma^2}\,\mathrm{d}(n^2) = \frac{h^2}{4ma^2} n \,\mathrm{d}n \tag{2.4.6}$$

Therefore we can substitute in:

$$\rho(E)\,\mathrm{d}E = \frac{\pi}{2} \underbrace{n}_{\sqrt{8ma^2E/h^2}} \underbrace{n\,\mathrm{d}n}_{4ma^2/h^2 \mathrm{d}E} = \frac{2\pi\left(2ma^2\right)^{3/2}}{h^3}\sqrt{E}\,\mathrm{d}E \tag{2.4.7}$$

and we can also express this wrt $p = \sqrt{2mE}$; its differential is $p\,\mathrm{d}p = m\,\mathrm{d}E$:

$$\rho(E)\,\mathrm{d}E = \rho(p)\,\mathrm{d}p = V\frac{4\pi a^3 p^2\,\mathrm{d}p}{h^3} \tag{2.4.8}$$

Where $a^3 = V$ is the volume, and since we treat a spherically symmetric problem we can rewrite it as $V = \frac{4}{3}\pi r_0^3 A$. Then, we put two fermions in each shell, thus getting N particles in total.

$$\mathrm{d}N = 2\rho(p)\,\mathrm{d}p = \frac{4}{3\pi}\frac{r_0^3 p^2}{\hbar^3} A\,\mathrm{d}p \tag{2.4.9}$$

Fermi sea This probability density must be normalized: let us consider the protons first. If their occupation is maximal up to p_F and null after, it must be

$$Z = \int_0^{p_F} 2\rho(p)\,\mathrm{d}p = \int_0^{p_F} \frac{4}{3\pi}\frac{r_0^3 p^2}{\hbar^3} A\,\mathrm{d}p = \frac{4A}{9\pi}\frac{r_0^3 p_F^3}{\hbar^3} \tag{2.4.10}$$

Turning this around gives

$$p_F c = \frac{\hbar c}{r_0}\sqrt[3]{\frac{9\pi}{8}\frac{2Z}{A}} \tag{2.4.11}$$

and we can find a similar result for the neutrons. Note that, if the nucleus is close to being symmetric, p_F only depends on $r_0 \propto \rho_0 = A/V$, not on A or V re

For light nucluei we can assume $2Z/A \approx 1$, and we know that $r_0 \approx 1.25\,\mathrm{fm}$. Then $p_F \approx 240\,\mathrm{MeV/c}$ and $E_F \approx 31\,\mathrm{MeV/c^2}$

If we assume that $V = E_F + B/A$ (as in, if we were to remove one nucleon at a time we would on average find them at the energy $-B/A$) we find that the potential well is around 40 MeV deep.

One more prediction of this model is that, for heavy nuclei with $N > Z$, $E_{F_N} > E_{F_P}$; the magnitude of the difference is around 32 vs 28 MeV for Uranium.

Isospin We consider nucleons as different manifestations of a single particle, with different eigenvalues for the z component of an operator $\vec{T}$, which has algebra $\mathfrak{su}(2)$. So, we assume that the nucleon is an isospin-1/2 particle (that is, the eigenvalue of T^2 is $3\hbar^2/4 = \hbar^2 i(i+1)$).

Average kinetic energy We have computed the state distribution differential $\mathrm{d}N$, with $\int \mathrm{d}N = A$ in equation (2.4.9). It is useful to split the neutron and proton contributions since in heavy nuclei their numbers differ significantly. For both of them we can find:

$$\langle E_k \rangle = \frac{1}{A}\int_0^A p^2/(2m)\,\mathrm{d}N = \frac{1}{A}\int_0^{p_F} \frac{p^2}{2m}\frac{4}{3\pi}\frac{r_0^3 p^2}{\hbar^3} A\,\mathrm{d}p = \frac{4}{3\pi}\frac{r_0^3}{\hbar^3}\int_0^{p_F}\frac{p^4}{2m}\,\mathrm{d}p \tag{2.4.12}$$

so adding their contributions we get

$$\langle E_k \rangle = \frac{4r_0^3}{3\pi\hbar^3}\left(\frac{p_{F_p}^5}{10m_p} + \frac{p_{F_n}^5}{10m_n}\right) \tag{2.4.13}$$

and we can substitute in the formula for the Fermi momentum (2.4.11), and approximate $m \approx m_n \approx m_p$: we get

$$\langle E_k \rangle = \frac{4r_0^3}{30m\pi\hbar^3}\left(\left(\frac{\hbar}{r_0}\sqrt[3]{\frac{9\pi}{8}\frac{2Z}{A}}\right)^5 + \left(\frac{\hbar}{r_0}\sqrt[3]{\frac{9\pi}{8}\frac{2(A-Z)}{A}}\right)^5\right) \tag{2.4.14a}$$

$$= \frac{3^{7/3}}{80}\frac{\pi^{2/3}\hbar^2}{80Amr_0^2}\left(\left(\frac{2Z}{A}\right)^{5/3} + \left(\frac{2(A-Z)}{A}\right)^{5/3}\right) \tag{2.4.14b}$$

Now, $2Z/A$ is approximately 1, so we can do a series expansion! $2Z/A \approx 1 + x$, where $x = (2Z - A)/A$.

We can use $(1+x)^{5/3} + (1-x)^{5/3} = 2 + 10x^2/9 + O(x^3)$. So,

$$\langle E_k \rangle = \frac{3^{7/3}}{80}\frac{\pi^{2/3}\hbar^2}{40Amr_0^2}\left(1 + \frac{5}{9}\left(\frac{2Z-A}{A}\right)^2\right) \tag{2.4.15}$$

2.5 Nuclear fission

Ellipsoid deformations The nucleus is approximately spherical, but we can model its oscillations as having an axis of rotational symmetry, thus having the shape of an ellipsoid. We call its two equal axes b and its different axis a. If $a > b$ the ellipsoid is prolate, otherwise it is oblate.

Since the volume is conserved, if $R = a = b$ is the spherical configuration, a small perturbation of it must look like $a = R(1+\varepsilon)$, $b = R(1+\varepsilon)^{-1/2}$.

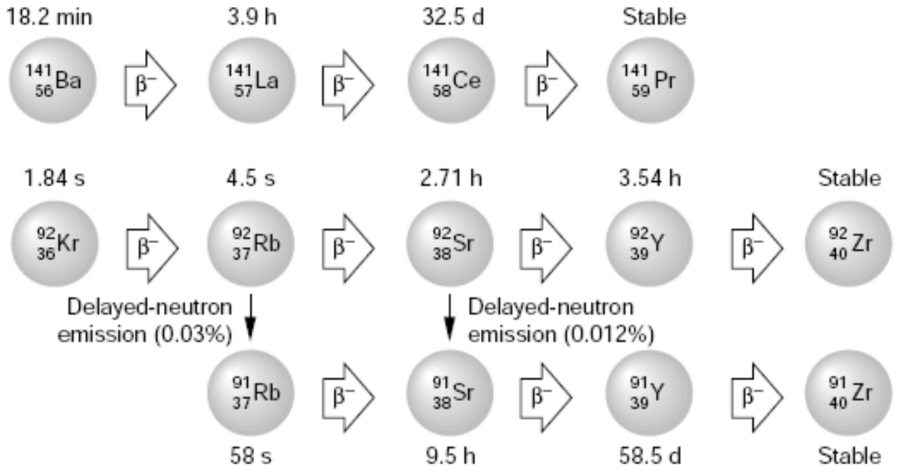


Figure 2.3: Barium decay chain

Calculations show that the surface increases like $4\pi R^2 \to 4\pi R^2\Big(1+(2/5)\varepsilon^2+O(\varepsilon^3)\Big)$, therefore $A^{2/3} \to \Big(1+(2/5)\varepsilon^2\Big)A^{2/3}$; we will also need the fact that $A^{-1/3} \to \Big(1-(1/5)\varepsilon^2\Big)A^{-1/3}$.

The part of the SEMF that changes looks like

$$B = -a_S A^{2/3} - a_C \frac{Z^2}{A^{1/3}} + \text{const} \to -a_S A^{2/3}\left(1+\frac{2}{5}\varepsilon^2\right) - a_C \frac{Z^2}{A^{1/3}}\left(1-\frac{1}{5}\varepsilon^2\right) + \text{const} \quad (2.5.1)$$

so we can compute the difference $B_{\text{new}} - B_{\text{old}} = \Delta B$:

$$\Delta B = A^{2/3}\left(-a_S\frac{2}{5}\varepsilon^2 + a_C\frac{Z^2}{A}\frac{1}{5}\varepsilon^2\right) = A^{2/3}\frac{\varepsilon^2}{5}\left(-2a_S + a_C\frac{Z^2}{A}\right) \quad (2.5.2)$$

this changes sign, becoming positive, for $a_S/a_C < Z^2/(2A)$. The ratio of the constants is known and approximately equal to $2a_S/a_C \approx 49$. At that point, becoming more elliptical corresponds to gaining energy, so the nucleus is unstable and will fission.

The inequality is reached around $Z \approx 114$, $A \approx 270$. This is not the limit seen experimentally: nuclei fission as early as $Z^2/A \approx 35$, but it gives a good theoretical justification of the fact that after a certain point we do not find any more stable nuclei.

Nuclear fission ^{235,238}U fission spontaneously, around 10^{-9} to 10^{-5} of the times they alpha-decay.

In fisssion from ^{238}U to $A \approx 119$ nuclei around 200 MeV of energy is emitted.

Neutron capture causing change in Z It works like this: the atom (say, ^{238}U) absorbs a neutron, becoming the excited ^{239*}U; then, this nucleus emits gamma radiation becoming ^{239}U, finally it balances the neutron excess by decaying β^- and thus becoming ^{239}Np.

Neutron capture causing fission The capture of a neutron can make an atom unstable wrt deformation, and then it might tunnel through the potential barrier.

Since the N/Z ratio is higher in heavier nuclei, the fission products will not be stable with the amount of neutrons they end up with, so they will tend to emit neutrons.

Some atoms have low energy barriers for fission, which can be surpassed by ambient temperature neutrons with $E = k_B T_{\text{amb}} \approx 26\,\text{meV}$ (^{235}U is like this), while others need fast-moving neutrons (like ^{238}U).

The probability of a nucleus of mass A being emitted in symmetric nuclear fission is bimodal, with high regions around $A \approx 90$ and $A \approx 130$.

2.6 Nuclear Fusion

Nuclear fission reactions can have very high energy yields, but also have high activation energies because of the Coulomb barrier.

$$Q = -\sum_{\text{reagents}} E_i + \sum_{\text{products}} E_i \tag{2.6.1}$$

Between the first nuclear fusion reactions one can write, the highest in Q is $\text{d} + \text{d} \to ^4\text{He} + \gamma$ with $Q \approx 24\,\text{MeV}$, while other reactions with protons and deutons have $Q = 3 \div 5\,\text{MeV}$.

Coulomb barrier Its height is

$$V_C = \frac{e^2}{4\pi\varepsilon_0}\frac{Z_1 Z_2}{R} \tag{2.6.2}$$

where R is the sum of the radii of the nuclei, a distance at which we assume the nuclear forces take over. For example, in the $\text{d} + \text{d}$ reaction, $V_C \approx 500\,\text{keV}$.

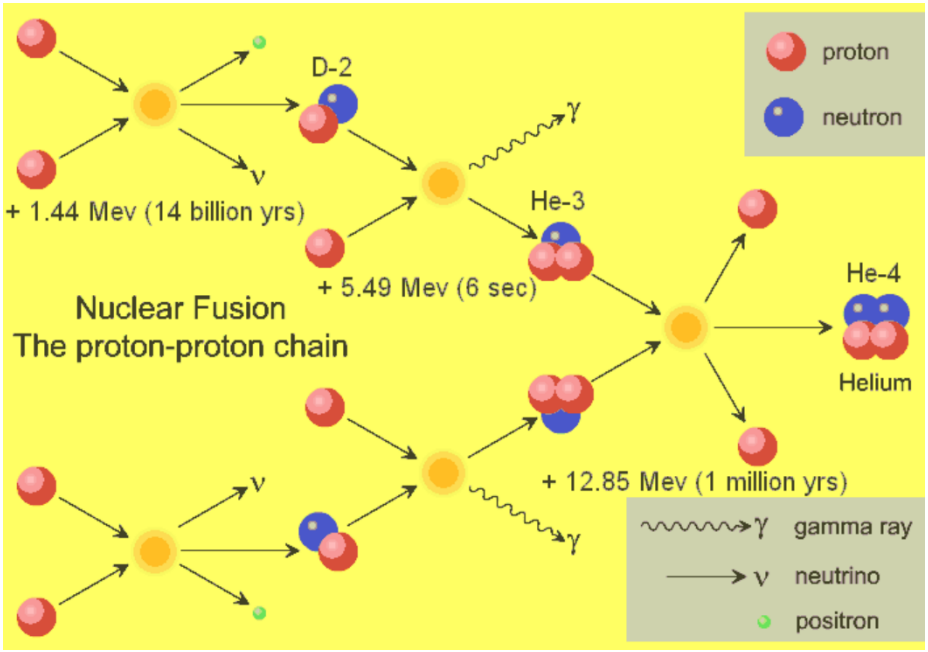


Figure 2.4: Nuclear decay chain in the Sun.

In figure 2.4 we show the nuclear fusion chain in the sun: from just protons we get ^{4}He, with a release of 26.73 MeV.

To get a high yield in nuclear fusion we need a kinetic energy on the order of 10 keV, which corresponds to very high temperatures.

2.7 Deuton

It is the only two-nucleon bound state; it has a *total* energy of 2.224 MeV

Its rms radius is around 2 fm, its spin-parity is $j^\pi = +1$, its magnetic moment is $\mu = 0.86\mu_N$.

It just has one degree of freedom, to study we only need the radial coordinate between the two nucleons: we assume our wavefunction to be in the form

$$\psi(r, \Omega) = \frac{u(r)}{r} Y_{ml}(\Omega) \tag{2.7.1}$$

where Ω is a pair of angles describing the relative position of the particles: $\vec{r} = (\vec{r_1} - \vec{r_2})/2$ is described by (r, Ω).

The radial part of the Schrödinger equation is

$$-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2 u}{\mathrm{d}r^2} + \left(V(r) + \frac{\hbar^2 l(l+1)}{2\mu r^2}\right)u(r) = Eu(r) \tag{2.7.2}$$

with $\mu = m_n m_p/(m_n + m_p) \approx m_p/2$. This comes from the fact that

$$P^2 = \frac{L^2}{r^2} - \hbar^2 \frac{1}{r}\frac{\partial^2}{\partial r^2} r \tag{2.7.3}$$

We model the potential as a well: then the (reduced) wavefunction u will look like $\sin(r)$ up to the end of the well, and $\exp(-r)$ after it, with wavevectors like $k_{\text{in}} = i\sqrt{2m(V_0 + E)/\hbar^2}$ and $k_{\text{out}} = \sqrt{-2m(E)/\hbar^2}$ as argument of the exponential.

Spin coupling The neutron and proton have either 0 or 1 as total spin S, and they are both even under spatial parity. The angular wavefunction has momentum L, and parity equal to $(-)^L$. Then, since we know that for the full deuton $j^\pi = +1$

$$(+)(+)(-)^L = (+) \qquad 1 = \vec{L} + \vec{S} \tag{2.7.4}$$

The first equation implies $L \in 2\mathbb{N}$. By the other, if $S = 0$ then $L = 1$, which cannot be. So $S = 1$, but this means $1 = \vec{1} + \vec{L}$, so $0 \leq L \leq 2$, therefore $L = 0, 2$.

By the Hund rule, we expect the state with the lower angular momentum ($^3\mathrm{S}_1$) to be the ground state.

With our newly found ground state we can compute expectation values, like the one of

$$\vec{\mu} = \frac{e\hbar}{2m}\vec{L} + \sum g_S \mu_N \vec{S} = (g_L^p + g_L^n)\mu_N \vec{L} + (g_S^p \vec{S_p} + g_S^n \vec{S_n})\mu_N \tag{2.7.5}$$

We know the values of the g factors.

In the ground state we expect $S = 0$, $L = 0$, and our particles have $s = 1/2$, therefore the expectation value will be $\langle\psi|\vec{\mu}|\psi\rangle = \frac{1}{2}(g_S^p + g_S^p)\mu_N$.

This is close to the true value but the measurement can be made very precisely, and the theoretical value does not hold up.

This is due to our hypothesis that the ground state is $|L = 0\rangle$ not being completely correct: the state is really a linear combination of mostly $|L = 0\rangle$ with a bit of $|L = 2\rangle$.

This suggest the existence of a tensorial term in the binding force, which mixes different angular momentum eigenstates. This is confirmed by the measurement of the quadrupole moment $Q \approx 3$ meb, which could not be nonzero if the ground state had only $L = 0$.

2.8 Shell model

Allows us to explain the magic numbers, and to model excited nuclear states.

We work assuming all but one of the nucleons just form the *core* with its mean field, and just work with the outermost nucleon in this mean field: $\hat{H}_{\text{single particle}} = p^2/2m + U_{\text{mean}}(r)$.

Evidence The plots of the separation energies for a neutron or a proton have dips at 1+ a magic number (of protons / of neutrons).

The residuals from the SEMF also have dips at magic numbers.

The magic numbers are 2, 8, 20, 28, 50, 82, 126. 40 is less magic.

Parabolic potential Our first idea is to Taylor expand the potential (wrt position): we have a constant term, the first derivative is zero, the second derivative gives us the harmonic term: so we have a Hamiltonian like $\hat{H} = \frac{1}{2m}p^2 + \frac{1}{2}mx^2\omega^2$.

Since it is a 3d oscillator, the energies look like $E_N = (N + \frac{3}{2})\hbar\omega$, with $N = \sum_i n_i$. This is in cartesian coordinates, in polars instead we can write $N = 2(n_r - 1) + L$, with $L \leq N$.

It can be shown with a group theory argument that the angular momentum must have the same parity as N.

Then the total degeneracy is

$$D(N) = \sum_{\substack{L \leq N \\ N+L \equiv 0 \bmod 2}} 2(2L+1) \tag{2.8.1}$$

since for every L we can have $2L+1$ values of L_z and for each of those two spin configurations.

This works up to around $Z = 20$, then we need to include some corrections.

Woods-Saxon potential It is a better approximation of the real potential than the parabolic one: it looks like the density function but with its sign flipped, so:

$$V_{\text{WS}} = \frac{-V_0}{1 + \exp\left(\frac{r - r_0}{a}\right)} \tag{2.8.2}$$

with $V_0 \approx 57\,\text{MeV}$, $r_0 \approx 1.25\,\text{fm}A^{1/3}$, $a \approx 0.65\,\text{fm}$.

Spin-orbital correction It is a perturbation to the total Hamiltonian of the form $L \cdot S = \frac{1}{2}\left(J^2 - L^2 - S^2\right)$ which, somewhat *ad hoc*, we multiply by a radial function.

$$E_{\text{spin-orbital}} = k\frac{\mathrm{d}V_{\text{WS}}}{\mathrm{d}r} L \cdot S \tag{2.8.3}$$

Other corrections The proton potential well will be higher than the neutron one, and it will have Coulomb tails.

There will also be an LL coupling term.

Excitations The number of possible excited states grows with A, because they depend on the j coupling. They can be formed in various ways: photoexcitation, inelastic scattering, or the nucleus can decay into an excited state.

How to calculate the ground state Look at figure 2.5 and start filling the neutron and proton shells separately. Hopefully you get to a configuration close to a full shell, then j^π can be calculated by looking at the single additional or missing nucleon(s).

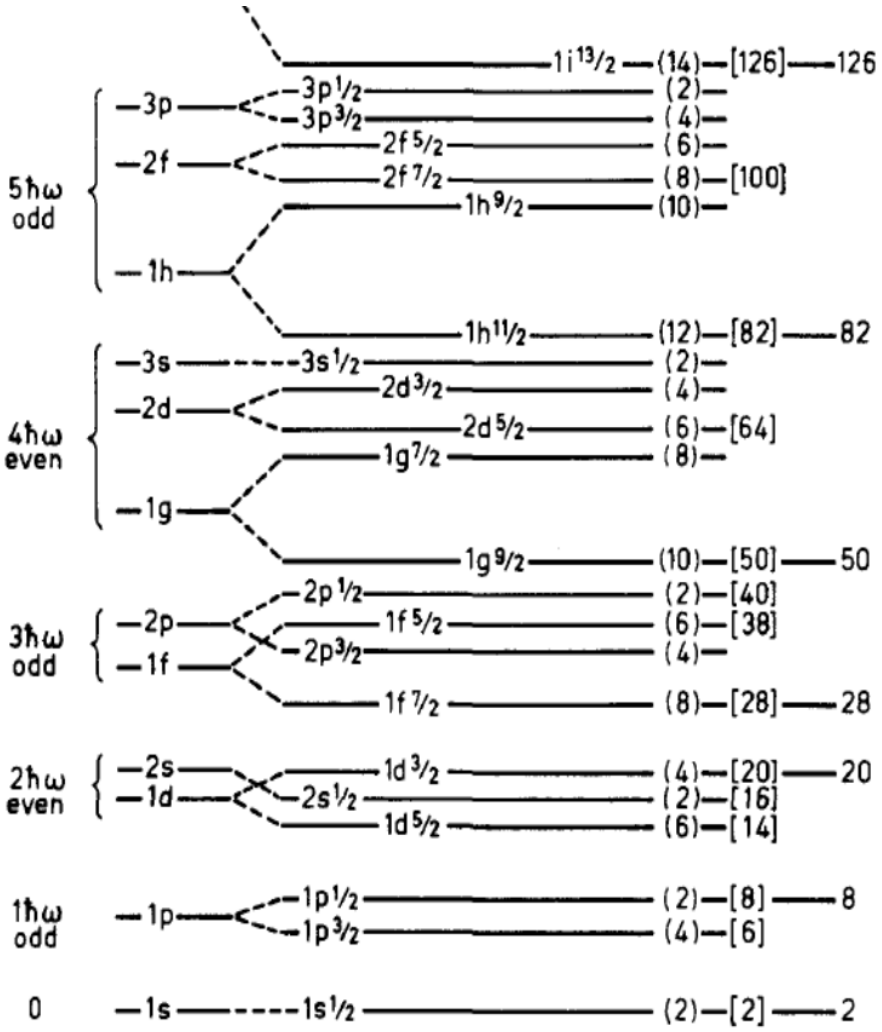


Figure 2.5: One-particle orbits

2.9 Collective model

It is used to describe the vibrations of the nucleus. In full generality, the angular distribution of the radius will look like

$$R(\theta,\varphi) = R_0\left(1+\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\alpha_{lm}Y_{lm}(\theta,\varphi)\right) \tag{2.9.1}$$

where the Y_{lm} are the normalized spherical harmonics (functions $Y : S^2 \to \mathbb{C}$ which satisfy $\nabla^2 Y = 0$, $L^2 Y_{lm} = \hbar^2 l(l+1)$, $L_z Y_{lm} = \hbar m$).

The term α_{00} is only relevant at very high energies (it is spherically symmetrical compression/expansion). The term α_{1m} correspond to translation, not an intrinsic vibration. So, we look at the quadrupole term, α_{2m}.

We can perform a rotation $\alpha_{2\mu} \to a_{2\mu}$ using the Wigner matrices[1] to go into a frame where $a_{21} = a_{2(-1)} = 0$ and $a_{22} = a_{2(-2)}$. We parametrize the nonzero as as $a_{20} = \beta\cos(\gamma)$, $a_{2(\pm 2} = \beta\sin(\gamma)/\sqrt{2}$. We used up 3 of the 5 dimensions for this.

The parameter $\beta = \sum |a_{2m}|^2$ describes the magnitude of the deformation, the parameter γ describes its direction: it can be shown that

$$R_k = R_0\left(1 + \frac{5}{4\pi}\beta\cos\left(\gamma + \frac{2}{3}\pi k\right)\right) \tag{2.9.3}$$

where $k = 1, 2, 3$.

We write the Hamiltonian of the oscillation with respect to the parameters $\alpha_{2\mu}$: the corresponding momenta are $\partial\Big/\partial\alpha_{2\mu} = \pi_{2\mu}$. Modelling the low-energy vibrations as a harmonic oscillator we get

$$H = \frac{\pi_{2\mu}\pi^\dagger_{2\mu}}{2B} + \frac{C}{2}\alpha_{2\mu}\alpha^\dagger_{2\mu} \tag{2.9.4}$$

and we have expressions for B, C.

The solutions for the Hamiltonian (2.9.4) can be shown to have energy $E = (\sum_\mu n_\mu + 5/2)\hbar\omega$, with $\omega = \sqrt{C/B}$. This formula implies the presence of degeneracy, but this is partially removed when introducing perturbations.

We can express the energy quantum number wrt the parameters β and γ: $\sum_\mu n_\mu = 2n_\beta + \tau$, where $\tau(\tau+3)$ is the eigenvalue of the Casimir operator on $SO(5)$.

2.10 α decay

α particles are ^{4}He nuclei. That configuration has a particularly high binding energy per nucleon. The reaction in α decay looks like

$${}^A_Z X \to {}^{A-4}_{Z-2} Y + \alpha \tag{2.10.1}$$

For it to happen, we must have $M(A,Z) > M(A-4,Z) + M(4,2)$. We can expand this in terms of the binding energies, and see that it will happen only for nuclei for which B/A is decreasing with A. The difference in energy between X and $Y + \alpha$ is denoted as Q. Since the velocities are not relativistic, the energy can be written as $Q = p_\alpha^2/2m_\alpha + p_Y^2/2m_Y$, and since $m_\alpha \ll m_Y$ but $|p_\alpha| = |p_Y|$ the energy is almost all kept by the α.

Different decays have wildly different half-lives: the empirical law they follow is called the *Geiger-Nuttal* (2.10.2). It is very closely followed if we fix an even Z and vary N keeping it even as well.

$$\log(t_{1/2}) \propto ZQ^{-1/2} \tag{2.10.2}$$

This can be understood with quantum tunneling. First of all, we assume the α can be spontaneously formed inside the nucleus as a cluster since it is a stable configuration, with some probability $\mathbb{P}_{\text{formation}} = \left|\langle\psi(A,Z)|\left(|\psi(A-4,Z-2)\rangle \otimes |\psi(4,2)\rangle\right)\right|^2$.

[1] They are the matrix elements of rotations with respect to the harmonics:

$$\mathcal{D}^j_{mm'}(\alpha,\beta,\gamma) = \left\langle jm'\right| \exp(-i\alpha J_z)\exp\left(-i\beta J_y\right)\exp(-i\gamma J_z)\left|jm\right\rangle \tag{2.9.2}$$

Then, this α will collide with the nucleus border at some rate, which we estimate as $f = 2r/v$. A very rough estimate gives $1/f \sim \hbar/\text{MeV} \approx 200\,\text{MeVfm}/(c\text{MeV}) \approx 10^{-21}\,\text{s}$.

So, we have to understand what happens at the nucleus border. We model the potential as a well, flat inside the nuclear radius R; outside, the α will feel the Coulomb repulsion of the nucleus

$$V(r) = \frac{e^2}{4\pi\varepsilon_0}\frac{Z_Y Z_\alpha}{r}[r \geq R] - V_0[0 \leq r < R] \tag{2.10.3}$$

Where $[\cdot]$ is the Iverson bracket.

The α can tunnel through the potential barrier: how likely is it to do so? Let us call this probability T. We can calculate it modelling our potential as many infinitesimal rectangular slices, let us also call $r = b$ the point at which $V(r) = Q$. Then,

$$T = \exp\left(-2\int_R^b \sqrt{\frac{2m(V(r)-Q)}{\hbar^2}}\,\mathrm{d}r\right) \tag{2.10.4}$$

since we know the wavefunction to be exponentially depressed as $\exp\left(-\Delta r\sqrt{2m(V-Q)/\hbar^2}\right)$ for a constant $V > Q$ and finite Δr, so we make Δr small and then we multiply together all the infinitesimal exponential probability decreases. The factor 2 comes from the fact that, to get the probabilities, we must take the square modulus.

This can be analytically calculated: if $T = \exp(-2G)$, then

$$G = 2\frac{Ze^2}{\hbar c}\sqrt{\frac{2m_\alpha c^2}{Q}}\left(\arccos\left(\sqrt{\frac{Q}{B}}\right) - \sqrt{\left(\frac{Q}{B}\right)\left(1-\frac{Q}{B}\right)}\right) \tag{2.10.5}$$

In the end, we can calculate the rate of decay as $\lambda = \mathbb{P}_{\text{formation}} T f$. As always, the decay law is $N(t) = N_0\exp(-\lambda t)$.

The orders of magnitude at play are as follows: $\mathbb{P}_{\text{formation}} \sim 1$, $f \sim 10^{21}\,\text{Hz}$, $G \sim 30 \div 50$.

2.11 β decay

A nucleon has its isospin flipped, emitting a $e^\pm$ and an electronic (anti)neutrino. This type of decay is due to the weak interaction.

Since it is a three-body process, we get a continuous spectrum of energies for the electron/positron.

Fermi theory Our assumptions are:

1. we neclect the Coulomb interaction between the electron and the nucleus (this will have to be reconsidered, since it only gives accurate predictions for $Z < 10$);
2. we neglect the recoil of the nucleus after the decay (the mass differences are very large: this will always work);
3. we assume $m_\nu = 0$;
4. we assume the distribution of energy partitions between the electron and neutrino to be uniform.

Fermi's golden rule The rate λ of a transition is given by

$$\lambda = \frac{2\pi}{\hbar}|M|^2\frac{\mathrm{d}n}{\mathrm{d}E} \tag{2.11.1}$$

where $M = \left\langle \psi_f \middle| H \middle| \psi_i \right\rangle$ is the matrix element between the initial and final states, H being the Hamiltonian due to which the transition happpens, $\mathrm{d}n/\mathrm{d}E$ is the differential phase volume corresponding to the energy E. Note that H is dimensional, it is an energy!

State density Recall the momentum dependence of the density of states from equation (2.4.8). Then

$$\mathrm{d}n = \left(\frac{4\pi V}{h}\right)^3 p_e^2\,\mathrm{d}p_e\,p_\nu^2\,\mathrm{d}p_\nu \tag{2.11.2}$$

The total energy is $E_0 = E_e + E_\nu$. We work at a fixed electron energy and momentum: so because of condition 3, $E_\nu = p_\nu c$, therefore $\mathrm{d}p_\nu = \mathrm{d}E_0\,/c$ and $p_\nu^2 = (E_0 - E_e)^2/c^2$. So we get

$$\mathrm{d}n = \left(\frac{4\pi V}{h}\right)^3 \frac{\mathrm{d}E_0}{c}\frac{(E_0 - E_e)^2}{c^2}p_e^2\,\mathrm{d}p_e \tag{2.11.3}$$

Calculation of λ We can plug this (with the $\mathrm{d}E_0$ brought to the left hand side) into equation (2.11.1), but we still have a differential to the right and we fixed p_e, so we will not obtain λ but the $\mathrm{d}\lambda$ from this momentum to $p_e + \mathrm{d}p_e$.

$$\mathrm{d}\lambda = \frac{2\pi}{\hbar}|M|^2\left(\frac{4\pi V}{h}\right)^3 F(Z_Y, E_e)\frac{(E_0 - E_e)^2}{c^3}p_e^2\,\mathrm{d}p_e = |M|^2\frac{(4\pi V)^3}{c^3h^4}F(Z_Y, E_e)(E_0 - E_e)^2p_e^2\,\mathrm{d}p_e \tag{2.11.4}$$

We get λ by integrating this expression. We also added a factor to account for the asymmetry between electrons and positrons: the former are slowed down by electrostatic attraction when leaving the nucleus, the latter are accelerated. So, we multiply λ by $F(Z_Y, E_e) = 2\pi\eta/(1 - \exp(-2\pi\eta))$, where $\eta = \mp\alpha Z_Y/\beta_e$, α being the fine-structure constant.

$$\lambda = |M|^2\frac{(4\pi V)^3}{c^3h^4}F(Z_Y, E_e)\int (E_0 - E_e)^2p_e^2\left[0 \le (p_ec)^2 \le E_0^2 - m_e^2c^4\right]\mathrm{d}p_e \tag{2.11.5}$$

Fermi-Kurie plot Flipping equation (2.11.4) around, we find that

$$K(E_e) = \sqrt{\frac{\mathrm{d}\lambda}{\mathrm{d}p_e}F^{-1}p_e^{-2}} \propto E_0 - E_e \tag{2.11.6}$$

a testable prediction, which is experimentally verified. Sometimes we get sums of different lines (in the limit in which the Ks are additive? maybe we can say that the $\mathrm{d}\lambda$s are additive and small so we make it work...).

If we had $m_\nu \neq 0$, the K plot would no longer be linear in E_e (instead of $p_\nu^2 = (E_0 - E_e)^2/c^2$ we would have had $p_\nu^2 = (E_0 - E_e)\sqrt{(E_0 - E_e)^2 - m_\nu^2c^4}/c^2$). This allows us to measure the neutrino mass.

From equation (2.11.5) we can calculate $ft \overset{\text{def}}{=} F(Z_Y, E_e)\log(2)/\lambda$. This is known as the ft value: it gives an estimate of $|M|^{-2}$. We usually plot its base-10 logarithm, since it varies through many orders of magnitude.

Calculating the matrix element We assume the interaction Hamiltonian is in the form $H = g\delta^3(r_e - r)\delta^3(r_\nu - r)$. In the calculation of M this will make all the integrals in the same variable, r. g's value cannot be determined theoretically, experimentally $g \approx 10^{-4}\,\mathrm{MeVfm}^3$. We must evaluate an expression as follows:

$$M = \int \psi_\nu^* \psi_e^* \psi_{\text{nuc - f}}^* \psi_{\text{nuc - i}}\,\mathrm{d}r \tag{2.11.7}$$

where all the wavefunctions are evaluated at r. If the electron and neutrino wavefunctions are planar waves, say $\psi_e = \exp(-ipr/\hbar) \sim 1 - ipr/\hbar + o(r)$. But we integrate only over the support of the nuclear wavefunctions: let us assume $r = r_0 A^{1/3} \approx 3 \div 5$ and $p = \sqrt{E_e^2/c^2 - m_e^2 c^2} \approx 1\,\mathrm{MeV/c}$. Then we see that the first order term is negligible. We do this for the electron and neutrino, getting $M = g\,\langle \text{nuc - f}|\text{nuc - i}\rangle\,/V$, where V is the volume we assume the electron and neutrino wavefunctions are normalized to have support in.

This is equivalent to assuming $p \wedge r = L = 0$ for the electron and neutrino.

Transition types We call the nuclear angular momentum I, the leptons' total angular momentum and spin L and S. Then

$$\vec{I_i} = \vec{I_f} + \vec{L} + \vec{S} \tag{2.11.8}$$

we distinguish

1. Fermi transitions: $S = 0$.
2. Gamow-Teller transitions: $S = 1$.

1. Permitted transitions: $\Delta L = 0$, they also have no change in parity since $\Delta\pi = (-)^{\Delta L}$. They are the ones we described in the last paragraph.
2. Super-permitted transitions: the starting and ending nuclear configurations are almost identical. This happens with specular nuclei. $\log_{10}(ft) \sim 3.5$.
3. Prohibited transitions (of various orders): every additional term in the expansion of the lepton wavefunctions depresses $|M|^2$ by a factor 10^4, so they get increasingly unlikely.

2.12 γ decay

γ radiation is almost monochromatic, since excited states usually live for around $10^{-12}\,\mathrm{s} \approx 1/6.6 \times 10^{-4}\,\mathrm{eV}$; its wavelength is also much longer than the nucleus.

The energy lost from the excited state is almost all with the γ: if we assume that energy and momentum are conserved we get $\Delta E = E_\gamma - E_\gamma^2/(2M)$ since $E_\gamma = p_{\text{recoil}}$. The solution of this is:

$$E_\gamma = M\left(-1 \pm \sqrt{1 + \frac{\Delta E}{M}}\right) \approx \Delta E - \frac{\Delta E^2}{M} \approx \Delta E \tag{2.12.1}$$

Selection rules We must have $\vec{I}_i = \vec{I}_f + \vec{L}$, and the angular momentum of the photon must be nonzero. Also, let us call EL the electric (due to moving charge) radiation with momentum L and ML the analogous magnetic (due to moving current) radiation. We call it 2^L-pole radiation. Then it can be shown that

$$EL \iff \Delta\pi = (-)^L \qquad ML \iff \Delta\pi = (-)^{L+1} \tag{2.12.2}$$

Emitted power Let us compare the emitted power to the first order of an electric dipole d vs a magnetic dipole μ, using the EM-fields formulas: $P(E1) \sim \omega^4 d^2/c^3$, while $P(M1) \sim \omega^4\mu^2/c^5$. In general, denoting $\sigma = E, M$:

$$P(\sigma L) = \frac{2c}{\varepsilon_0}\frac{(L+1)}{L((2L+1)!!)^2}\left(\frac{\omega}{c}\right)^{2L+2}\mathcal{M}(\sigma L)^2 \tag{2.12.3}$$

where $\mathcal{M}$ can be interpreted, in a quantum setting, as a *transition amplitude*, whose square modulus is a transition probability. To calculate $\mathcal{M}$ we should use the multipole operators, which for the electric transitions are $O(EL) = er_i^L Y_{i,LM}$ (i labels the particles in the nucleus) while the magnetic ones are much more complicated.

In general, $\mathcal{M}(\sigma L) = \left\langle \psi_f \right| O(\sigma L) \left| \psi_i \right\rangle$. Dimensionally, $[\mathcal{M}] = Cm^L$.

We can find the rate of photon emission as $T(\sigma L) = P(\sigma L)/\hbar\omega$.

$$T(\sigma L) = \frac{8\pi\alpha c(L+1)}{e^2 L(2L+1)!!^2}\left(\frac{\omega}{c}\right)^{2L+1}\left|\mathcal{M}(\sigma L)\right|^2 \tag{2.12.4}$$

Weisskopf estimations Instead of the multipole operators, we use brutal estimates (the radial wavefunctions are proportional to $[r \in \text{nucleus}]$, the angular integrals are 1):

$$\left|\mathcal{M}(EL)\right|^2/e^2 = \frac{1}{4\pi}\left(\frac{3}{3+L}\right)^2 (r_0 A^{1/3})^{2L} \tag{2.12.5a}$$

$$\left|\mathcal{M}(ML)\right|^2 \propto \left(\frac{3}{3+L}\right)^2 (r_0 A^{1/3})^{2L-2} \tag{2.12.5b}$$

The ratio of the magnetic to electric matrix square element is something like $0.31A^{-2/3} \sim 10^{-2}$. The take-away is: when L increases by 1, the transition probability decreases by a factor $10^4 \div 10^5$.

In the end, setting $R = r_0 A^{1/3}$, we get

$$T(EL) \approx \frac{2\alpha(L+1)}{L(2L+1)!!^2}\left(\frac{\omega}{c}\right)^{2L+1}\left(\frac{3}{3+L}\right)^2 R^{2L} \tag{2.12.6}$$

Around magic numbers this prediction is close to being verified; mid-shell we see tens or hundreds more than it. The half-life of the decay is given by $t_{1/2} = \log(2)/T$

Experimental methods We can experimentally determine the parity of a Γ transition: we look at the differential cross section $\mathrm{d}\sigma/\mathrm{d}\theta$ wrt the azimuth angle θ, if it is odd then the change in parity is $(-)$, if it is even the change in parity is $(+)$.

Also, we can look at the number of nodes $\mathrm{d}\sigma/\mathrm{d}\theta$, which will be equal to the order of the Legendre polynomial of the radiation.

2.13 Matter and radiation

Cross sections The flux of particles $\varphi = \#\text{particles}/(At) = nv$ (where A is the area through which the particles pass, t is the time interval, n is the particle density and v is the velocity) decays like $\Delta\varphi = -\varphi\sigma n_t \Delta x$, where n_t is the particle density in the target, and the proportionality constant σ [m^2] is called the scattering cross section.

There are three types of interaction between photons and matter. Photoelectric is dominant at low energies, Compton at mid energies, pair production at high energies. As Z of the material increases, the Compton-dominance region shrinks (on a log plot, somewhat symmetrically around 1 MeV).

Photoelectric : $\sigma \sim Z^{4\div5}/E_\gamma^3$, for $E_\gamma < 400\,\text{keV}$.

Compton : continuous spectrum,

$$E'_\gamma = \frac{E_\gamma}{1 + (E_\gamma/m_e c^2)(1-\cos(\theta))} \qquad \text{or} \qquad \frac{1}{E'_\gamma} - \frac{1}{E_\gamma} = \frac{m}{1-\cos(\theta)} \tag{2.13.1}$$

Remember: the initial electron mass goes into the energy count! The maximum energy transferred to the electron is at $\theta \to \pi$, $E'_\gamma - E_\gamma \to m_e c^2/2$.

Pair production Near a nucleus, we can have some momentum transfer and see $\gamma \to e^- + e^+$.

α particle energy transfer The collision is elastic and the α's mass is much larger than the electron's: the energy transferred is approximately

$$E_e = \frac{4 m_e E_\alpha}{M_\alpha} \tag{2.13.2}$$

so, for a regular α, in the single keV range.

Bethe-Bloch It describes the *stopping power* $\mathrm{d}E/\mathrm{d}x$ of a particle in a medium. We use the following assumptions: the particle has mass M, charge ze, velocity v, the impact parameter wrt the medium electrons is b, the material has Z, A. Imagine a very long cylinder centered around the particle: by Gauss, ignoring the circular faces,

$$\frac{ze}{\varepsilon_0} = \int E_\perp \,\mathrm{d}x\, b\,\mathrm{d}\theta = \int eE 2\pi b\,\mathrm{d}x \tag{2.13.3}$$

The momentum transferred to the electron is the integral of $\mathrm{d}p_\perp = F_\perp\,\mathrm{d}t = eE_\perp\,\mathrm{d}t$. Also, recall $\mathrm{d}t = \mathrm{d}x\,/v$. Then

$$\Delta p_\perp = \int eE\,\mathrm{d}t = \int eE \frac{2\pi b}{2\pi b}\frac{\mathrm{d}x}{v} = \frac{ze}{\varepsilon_0}\frac{e}{2\pi b v} \tag{2.13.4}$$

So, at fixed b and electron position, we can calculate $\Delta E = \Delta p^2/2m_e$.

But this will hold for all the electrons, and there are N of them, so $\Delta E_{\text{tot}} = N\Delta E$. We can write $N = nV$. If we have the density ρ, the (approximate) molar mass A, then $n = ZN_A\rho/A$ since there are Z electrons per atom. Also, $V = \int 2\pi b\,\mathrm{d}b\,\mathrm{d}x$.

Putting it all together, and calculating the energy difference for the particle, which is minus that of the electron:

$$-\Delta E = \int \left(\frac{ze}{\varepsilon_0}\frac{e}{2\pi b v}\right)^2 \frac{1}{2m_e}\frac{ZN_A\rho}{A} 2\pi b \,\mathrm{d}b\,\mathrm{d}x \tag{2.13.5a}$$

$$-\frac{\mathrm{d}E}{\mathrm{d}x} = \left(\frac{ze^2}{4\pi\varepsilon_0}\right)^2 \frac{4\pi Z N_A \rho}{m_e v^2 A}\int \frac{\mathrm{d}b}{b} \tag{2.13.5b}$$

$$-\frac{\mathrm{d}E}{\mathrm{d}x} = \left(\frac{ze^2}{4\pi\varepsilon_0}\right)^2 \frac{4\pi Z N_A \rho}{m_e v^2 A}\log\left(\frac{m_e v^2}{h\left\langle \nu_e\right\rangle}\right) \tag{2.13.5c}$$

where we used $b_{\max} = 2v/\left\langle \nu_e\right\rangle$, since if the time it takes the electron to oscillate ($1/\left\langle \nu\right\rangle$) is larger than the time it takes the interaction to occur ($b/2v$, half of the path of the particle) then the electron will not behave as a point particle; also $b_{\min} = h/p_e = h/(m_e v)$ since then the particle will pass *through* the electron, and quantum stuff will happen. We introduce $I = h\left\langle \nu\right\rangle$ as the ionization potential of the material, and some terms coming from relativistic considerations

$$S = -\frac{\mathrm{d}E}{\mathrm{d}x} = \left(\frac{ze^2}{4\pi\varepsilon_0}\right)^2 \frac{4\pi Z N_A \rho}{m_e v^2 A}\left(\log\left(\frac{2m_e v^2}{I(1-\beta^2)}\right) - \beta^2\right) \tag{2.13.6}$$

for energies between 100 keV and 1 GeV, the shape of the curve is roughly $S \propto E^{-0.8}$.

Range It is the distance travelled by the particle: we can compute it as

$$R = \int \frac{\mathrm{d}x}{\mathrm{d}E}\,\mathrm{d}E = \int_0^{E_0} \frac{\mathrm{d}E}{-S} \tag{2.13.7}$$

plugging in a rough version of formula (2.13.6) (we get this by dividing and multiplying by M, the mass of the particle): $S \approx azE^{-1} = 2azM/E$. Then

$$R \approx \frac{1}{2a}\frac{E_0^2}{z^2 M} \tag{2.13.8}$$

Chapter 3

Quantum Information

3.1 The basics

Qubit It can be physically realized with any two-state system. It is a complex superposition of $|0\rangle$ and $|1\rangle$. Thanks to normalization and $U(1)$ gauge invariance (a ket is defined up to a phase) we can always make $|0\rangle$'s coefficient real and $\in [0,1]$: the ket can always be written as

$$|\psi\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + \sin\left(\frac{\theta}{2}\right)e^{i\varphi}|1\rangle \tag{3.1.1}$$

with $\varphi \in [0, 2\pi]$ and $\theta \in [0, \pi]$: these can be interpreted as angles on a sphere. The fact that θ is divided by two comes from the coordinates we choose in $S^3 \subset \mathbb{C}^2$.

We can use an n-qubit system:

$$|\psi\rangle = \sum_{i=0}^{2^n-1} a_i |i\rangle \tag{3.1.2}$$

where $|i\rangle$ is a base state of the tensor product space of the n Hilbert spaces: $|i\rangle = |\alpha_0\rangle_0 \otimes |\alpha_1\rangle_1 \otimes \ldots |\alpha_{n-1}\rangle_{n-1}$; the α_j are the components of the representation of i in binary: $\alpha_0\alpha_1\ldots\alpha_{n-1}$ (with $\alpha_j = 0, 1$). This is called the *computational basis*.

We assume the state to be normalized: $\sum_i |a_i|^2 = 1$

Entanglement A state $|\psi\rangle$ is called *entangled* if there are no subsystem kets $|\psi_i\rangle_i$, $i = A, B$ such that $|\psi\rangle = |\psi_A\rangle_A \otimes |\psi_B\rangle_B$.

3.2 Quantum gates

They are unitary trasformations: $U : \mathcal{H} \to \mathcal{H}$, $U^\dagger U = UU^\dagger = \mathbb{1}$.

They can be decomposed into smaller gates, which are in general $2n \times 2n$ complex unitary matrices, but we will usually just use $n = 1, 2$.

If two gates are represented by 2×2 matrices, indexed in the computational basis as A_i^j and B_k^l with $i, j, k, l = 0, 1$, then their tensor product will be

$$[A_i^j B_k^l] = [A \otimes B]_{i\,k}^{j\,l} = [A \otimes B]_M^N \tag{3.2.1}$$

where we grouped the indices $ik = M$ and $jl = N$, in order to write two-component fourth order tensors as four-dimensional order two matrices. What are M and N then? i, j and so on are binary digits, so it is natural to interpret M and N as numbers between 0 and 3 written

in binary. Of course, this can be generalized to any order, keeping the same pattern, and be applied to vectors as well.

Hadamard It is a *one-qubit gate* which switches from the computational basis to the eigenstates of σ_z, which we call $|+\rangle = H|0\rangle \propto |0\rangle + |1\rangle$ and $|-\rangle = H|1\rangle \propto |0\rangle - |1\rangle$.

$$H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \tag{3.2.2}$$

We can also express it, for the basis states, as $H|x\rangle = \sqrt{1/2} \sum_{y=0}^{1} (-)^{xy} |y\rangle$.

Phase It is a *one-qubit gate* which gives a phase to a state: applying it to a generic qubit, written as (3.1.1), we get $R_z(\delta)|\psi\rangle = \cos(\theta/2)|0\rangle + \exp\big(i(\varphi+\delta)\big)\sin(\theta/2)|1\rangle$.

$$R_z(\delta) = \exp(i\delta\sigma_z) = \begin{bmatrix} 1 & 0 \\ 0 & \exp(i\delta) \end{bmatrix} \tag{3.2.3}$$

Control not It is a *two-qubit gate* which cannot be written as a tensor product of one-qubit gates.

$$\text{CNOT} = \begin{bmatrix} 1 & 0 & & \\ 0 & 1 & & \\ & & 0 & 1 \\ & & 1 & 0 \end{bmatrix} \tag{3.2.4}$$

It generates entanglement: let us apply it to the separable state $\alpha|00\rangle + \beta|10\rangle$: it returns $\alpha|00\rangle + \beta|11\rangle$, which is entangled.

Control phase It is a *two-qubit gate*:

$$\text{CPHASE}(\delta) = \begin{bmatrix} \mathbb{1} & 0 \\ 0 & R_z(\delta) \end{bmatrix} \tag{3.2.5}$$

where we used the phase gate (3.2.3).

It can be written as $\text{CPHASE}(\delta) = [\mathbb{1} \otimes R_z(\delta/2)][\text{CNOT}][\mathbb{1} \otimes R_z(-\delta/2)][\text{CNOT}][R_z(\delta/2) \otimes \mathbb{1}]$: the steps (multiplying from right to left, starting from just $[R_z(\delta/2) \otimes \mathbb{1}]$) are as follows:

$$\begin{bmatrix} 1 & & & \\ & 1 & & \\ & & e^{i\delta/2} & \\ & & & e^{i\delta/2} \end{bmatrix} \to \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & & e^{i\delta/2} \\ & & e^{i\delta/2} & \end{bmatrix} \to \begin{bmatrix} 1 & & & \\ & e^{-i\delta/2} & & \\ & & & e^{i\delta/2} \\ & & 1 & \end{bmatrix} \to$$
$$\to \begin{bmatrix} 1 & & & \\ & e^{-i\delta/2} & & \\ & & 1 & \\ & & & e^{i\delta/2} \end{bmatrix} \to \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & e^{i\delta} \end{bmatrix} \tag{3.2.6}$$

We can get any state $|\psi\rangle$ written as (3.1.1) with Hadamard and phase-shift:

$$|\psi\rangle = R_z(\pi/2+\varphi)HR_z(\theta)H|0\rangle \tag{3.2.7a}$$

$$= \frac{1}{2}\begin{bmatrix} 1+e^{i\theta} \\ i\left(e^{i\varphi} - e^{i(\theta+\varphi)}\right) \end{bmatrix} \tag{3.2.7b}$$

$$= \frac{1}{2}\begin{bmatrix} e^{i\theta/2} + e^{-i\theta/2} \\ i^{-1}\left(e^{i\theta/2} - e^{-i\theta/2}\right)e^{i\varphi} \end{bmatrix} \tag{3.2.7c}$$

$$= \begin{bmatrix} \cos(\theta/2) \\ \sin(\theta/2)e^{i\varphi} \end{bmatrix} \tag{3.2.7d}$$

where in the step (3.2.7c) we used the fact that a quantum state is only defined up to a phase, and multiplied by $\exp(-i\theta/2)$.

Binary function unitarity In general a function $f : \{0,1\}^n \to \{0,1\}$ will not be injective, therefore it will not be unitary. In order to represent it as unitary we must "carry over" the input:

$$U_f|x\rangle|0\rangle = |x\rangle|f(x)\rangle \tag{3.2.8}$$

in order to have a more general trasformation we define it for arbitrary input on the second system:

$$U_f|x\rangle|y\rangle = |x\rangle|y \oplus f(x)\rangle \tag{3.2.9}$$

where $\oplus$ is bitwise XOR.

Parallelism We can do lots of computation with a single gate: say we have a state like (3.1.2), then

$$U_f \sum_{x=0}^{2^n-1} a_x|x\rangle|y\rangle = \sum_{x=0}^{2^n-1} a_x|x\rangle|y \oplus f(x)\rangle \tag{3.2.10}$$

For this to be really different from classical computing, however, a significant portion of the 2^n coefficients a_x must be nonzero. We now will show how to produce the state in which they are all equal to $2^{-n/2}$, assuming we can produce $|0\rangle^{\otimes n}$. We apply a Hadamard gate to every qubit, which carries a normalization and a factor of $(-)^{x_i y_i}$, so we get:

$$H^{\otimes n}|x\rangle = \frac{1}{\sqrt{2^n}} \sum_{y=0}^{2^n-1} (-)^{x\cdot y}|y\rangle \tag{3.2.11}$$

And the desired state can be found by setting $x = 0$. Do note that while this looks "entangled" we found it by applyng single-qubit gates: it is still separable (we can see this from the fact that its density matrix has the same value in every entry, so its rank is 1).

No cloning A *general* cloning unitary operator would look like: $U|x\rangle|0\rangle = |x\rangle|x\rangle$. Let us assume we have one, and let us apply it to two different states: $A = U|\psi\rangle|0\rangle = |\psi\rangle|\psi\rangle$ and $B = U|\varphi\rangle|0\rangle = |\varphi\rangle|\varphi\rangle$. Now, let us compute the scalar product of A and B:

$$\begin{aligned} A \cdot B &= \langle\psi|\langle 0|U^\dagger U|\varphi\rangle|0\rangle && \text{(3.2.12a)} \\ &= \langle\psi|\varphi\rangle\langle 0|0\rangle U^\dagger U && \text{(3.2.12b)} \\ &= \langle\psi|\varphi\rangle && \text{(3.2.12c)} \end{aligned}$$

but also

$$\begin{aligned} A \cdot B &= \langle\psi|\langle\psi||\varphi\rangle|\varphi\rangle && \text{(3.2.13a)} \\ &= \langle\psi|\varphi\rangle^2 && \text{(3.2.13b)} \end{aligned}$$

and in general $\langle\psi|\varphi\rangle \neq 0, \pm 1$, so we found a contradiction. Note that we *can* create a partial cloning machine which works only on the basis states of some basis: we extend by linearity the desired cloning. If we want to clone the computational basis, the gate is the CNOT (see 'Control not' on page 49).

Alternative proof: apply $U(|x\rangle + |y\rangle) \otimes |0\rangle = (|x\rangle + |y\rangle)^{\otimes 2}$ (a separable state), but U must be linear, so $U(|x\rangle + |y\rangle) \otimes |0\rangle = |x\rangle|x\rangle + |y\rangle|y\rangle$, generally an entangled state.

3.3 Miscellaneous concepts

3.3.1 Algorithmic complexity

We can distinguish algorithms by how many resources (computation time, RAM, ...) they require:

1. P: classical polynomial time;
2. NP: classical nondeterministic polynomial time: there exists a nondeterministic Turing machine[1] which finds the solution in polynomial time — the solution can thus be verified in polynomial time;
3. $NP-$hard: problems to which every P problem can be reduced in polynomial time;
4. NPC: NP problems which are also $NP-$hard;
5. BPP: bounded error probabilistic polynomial: it can give us the correct answer in polynomial time with probability $\mathbb{P} > 1/2$.
6. BQP: bounded error quantum polynomial: it is a quantum algorithm which can give us the correct answer in polynomial time with probability $\mathbb{P} > 1/2$.

Surely $P \subseteq BPP \subseteq BQP$. We are not sure whether $BQP \subseteq BPP$.

[1] Same as a regular Turing machine, except that in a certain configuration it can have different actions, and in a certain sense it "tries them all".

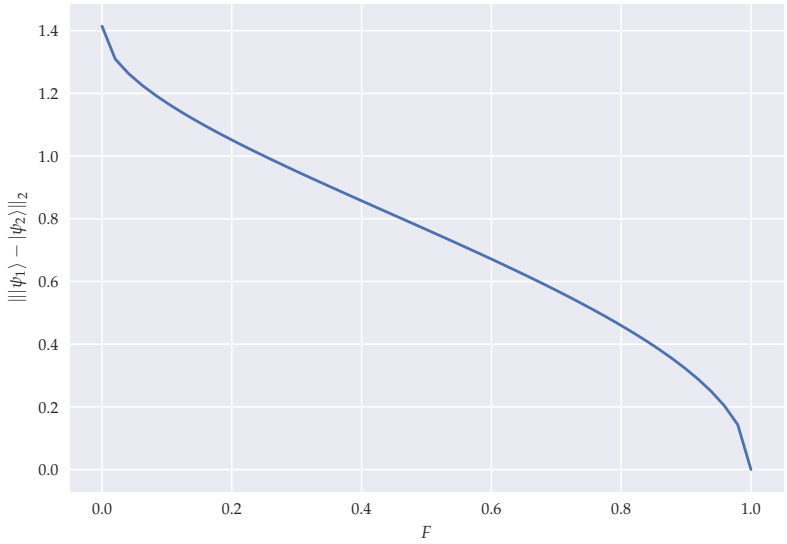


Figure 3.1: Norm of difference vs fidelity: a plot of equation (3.3.2)

3.3.2 Fidelity

We introduce a notion of distance between states:

$$F = \left| \langle \psi_1 | \psi_2 \rangle \right|^2 \tag{3.3.1}$$

F is monotonous in $\left\| |\psi_1\rangle - |\psi_2\rangle \right\|_2$. F is also the $\cos^2(\theta/2)$, where θ is the angle between the two vectors in Bloch space.

Let us prove these two statements: first of all notice that $\left\| |\psi_1\rangle - |\psi_2\rangle \right\|_2 = \sqrt{2 - 2\,\mathrm{Re}\,\langle \psi_1 | \psi_2 \rangle}$. Now, the scalar product $\langle \psi_1 | \psi_2 \rangle$ is in general a complex number but we can rotate the starting functions by an arbitrary phase, making it real and positive. So we get $\mathrm{Re}\,\langle \psi_1 | \psi_2 \rangle = \left| \langle \psi_1 | \psi_2 \rangle \right| = \sqrt{F}$. Then, we can see that

$$\left\| |\psi_1\rangle - |\psi_2\rangle \right\|_2 = \sqrt{2(1 - \sqrt{F})} \tag{3.3.2}$$

Now, we want to prove $F = \cos^2(\theta/2)$: let U be a unitary transformation which maps $|\psi_1\rangle$ to $|0\rangle$. We can rewrite $F = \left| \langle \psi_1 | U^\dagger U | \psi_2 \rangle \right|^2$. We can expand the applications of U to the vectors to get $\left| \langle 0 | \left(\alpha |0\rangle + \beta |1\rangle \right) \right|^2$.

Now, since states are always defined up to a phase, we can pick α to be real and positive. Then we have put the state $U |\psi_1\rangle$ in the canonical form (3.1.1), and the result follows.

3.4 Quantum teleportation

It is possible to clone a generic quantum state $|\psi\rangle = \alpha |0\rangle + \beta |1\rangle$ assuming we start with two entangled qubits, one in the starting location and one at the destination: so, if these two qubits are called A and B and the state we want to transmit is in subsystem C, we start with

$$\left(\frac{|00\rangle + |11\rangle}{\sqrt{2}}\right)_{AB} \otimes |\psi\rangle_C \tag{3.4.1}$$

The protocol is this:

1. Apply the gate $C_C NOT_A$;
2. apply the gate H_C;
3. measure A and C in the computational basis: call the result x;
4. apply a gate V_x, selected according to table 3.1, to B.

x	V_x
00	$\mathbb{1}$
01	σ_z
10	σ_x
11	$\sigma_z\sigma_x$

Table 3.1: Possibilities for gate V_x.

Possibly, when Montangero wrote $AC = 01$ he meant $A = 1$ and $C = 0$.

We can realize all of this with the gates CNOT, Hadamard and σ_z (we can recover σ_x as $\sigma_x = H\sigma_z H$.

3.5 Quantum interferometry

Beam splitter We call the sides of the BS A and B, and denote the absence or presence of light on either side by $|0,1\rangle_{A,B}$. Then the action of the beam splitter is unitary and can be represented in the partial basis $|0\rangle_A \otimes |1\rangle_B, |1\rangle_A \otimes |0\rangle_B$ as

$$U_{BS} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & i \\ i & 1 \end{bmatrix} \tag{3.5.1}$$

Note that $U_{BS}^2 = i\sigma_x$ in the BS-side basis: if we build a Mach-Zender interferometer, that is, we chain two beam-splitters, the light from the two paths interferes and we get some only on one side of the BS (the side opposite of the starting one).

Bomb detection If we block one of the paths between the detectors, around half of the time the light will hit this obstacle (our 'bomb'). Around half the time it will go to the second BS, and then a quarter of the time it will be detected on either side of the BS. On the other hand, if there is no obstacle, we will see photons *only* on a certain side of the final BS.

So around $1/4$ of the time we will have detected the bomb without the photon actually *having been there*.

3.6 Zeno effect

We will work with $\hbar = 1$. We look of the *survival probability* with which we will retain our starting state: if our evolution operator is $U = \exp(-iHt)$, this probability is $\mathbb{P} = A^*A$, where $A = \langle\psi_0|\psi(t)\rangle$ and $|\psi(t)\rangle = U|\psi_0\rangle$.

How does this probability look like for small t? We can expand, for a small δt:

$$U \sim \mathbb{1} - iH\delta t - H^2\delta t^2 \tag{3.6.1}$$

then we will have

$$A = \langle\psi_0|\left(\mathbb{1} - iH\delta t - H^2\delta t^2\right)|\psi_0\rangle = 1 - i\langle H\rangle_0\,\delta t - \frac{1}{2}\left\langle H^2\right\rangle_0\delta t^2 \tag{3.6.2}$$

so we can calculate $\mathbb{P}$:

$$\mathbb{P} = \left|1 - i\langle H\rangle_0\,\delta t - \frac{1}{2}\left\langle H^2\right\rangle_0\delta t^2\right|^2 = 1 - \delta t^2\left(\left\langle H^2\right\rangle_0 - \langle H\rangle_0^2\right) \tag{3.6.3}$$

Equation (3.6.3) is accurate to the order δt^3, since we only ignored a fourth order term. The term multiplying δt^2 can be interpreted as the inverse of a characteristic time:

$$\tau = \frac{1}{\sqrt{\langle H^2\rangle_0 - \langle H\rangle_0^2}} = \frac{1}{\Delta H_0} \tag{3.6.4}$$

Repeated measurements If we measure some observable with $|\psi_0\rangle$ as an eigenspace, a fraction t^2/τ^2 of the time we will get something different from $|\psi_0\rangle$.

So, if in a long time t we measured N times, the probability of the system having remained in the original state is at least $\mathbb{P}(t) \geq \mathbb{P}^N(t/N)$: we consider the case in which the system remained in the state for *all* the measurements. The latter pertains to a small time so we can apply equation (3.6.3):

$$\mathbb{P} \geq \mathbb{P}^N\left(\frac{t}{N}\right) = \left(1 - \frac{t^2}{N^2\tau^2}\right)^N \tag{3.6.5}$$

if we fix the inverse of the measurement rate $N/t = R$ this becomes $\mathbb{P} \geq x^t = \exp\big(t\log x\big)$, with $x = (1 - 1/R^2\tau^2)^R$, so $\log x = R\log(1 - 1/R^2\tau^2) < 0$. So, we call $-\log x = \gamma_{\text{eff}} > 0$: then

$$\mathbb{P} \geq e^{-\gamma_{\text{eff}}t} \tag{3.6.6}$$

Note that as $R \to \infty$, $\gamma_{\text{eff}} \sim R^{-1}\tau^{-2}$.

An example of nonunitary evolution We consider a Hamiltonian like $H = \Omega\sigma_x$, which might be that of a spin-1/2 particle, polarized along z, in a magnetic field along x. Say our system starts at $|\psi_0\rangle = |0\rangle$. Then the evolution looks like

$$\exp(-iHt)\,|0\rangle = \cos(\Omega t)\,|0\rangle - i\sin(\Omega t)\,|1\rangle \tag{3.6.7}$$

We can calculate the quantities from section 3.6: $A = \cos(\Omega t)$ and $\mathbb{P} = \cos^2(\Omega t)$, for small t: $\mathbb{P} \sim 1 - \Omega^2 t^2$. We recognise the expression for the Zeno time: in this case $\tau = \Omega^{-1}$

Let us introduce the nonunitary part: we change H to

$$H_{\text{int}} = \begin{bmatrix} -iV \\ \Omega \\ 0 \\ +iV \end{bmatrix} \cdot \begin{bmatrix} \mathbb{1} \\ \sigma_x \\ \sigma_y \\ \sigma_z \end{bmatrix} = -iV\mathbb{1} + \vec{h}\cdot\vec{\sigma} = \begin{bmatrix} 0 & \Omega \\ \Omega & -2iV \end{bmatrix} \tag{3.6.8}$$

to represent interaction with a second lower-energy system, to which our first one can decay *if it is in the state* $|1\rangle$. Can we get a Zeno-like effect with this kind of interaction, and without *measuring* anything? The evolution of this new Hamiltonian will look like

$$\exp(-itH) = e^{-tV}\exp\left(-it\vec{h}\cdot\vec{\sigma}\right) = e^{-tV}\left(\cosh(ht)\mathbb{1} - i\frac{\vec{\sigma}\cdot\vec{h}}{h}\sinh(ht)\right) \tag{3.6.9}$$

where $h = \sqrt{V^2 - \Omega^2} \in \mathbb{R}$, since we assume the coupling is strong ($V \gg \Omega$).

This comes from the fact that for a unit vector $\vec{n}$: $(\vec{n}\cdot\vec{\sigma})^n = \mathbb{1}$) if N is odd, $\vec{n}\cdot\vec{\sigma}$ otherwise: thus we can show that

$$\exp\big(i\theta(\hat{n}\cdot\sigma)\big) = \cos(\theta)\mathbb{1} + i(\hat{n}\cdot\sigma)\sin(\theta) \tag{3.6.10}$$

So, we can compute $A = \langle U\rangle_0$:

$$A = \frac{1}{2}\left(1 + \frac{V}{h}\right)e^{-(V-h)t} + \frac{1}{2}\left(1 - \frac{V}{h}\right)e^{-(V+h)t} \tag{3.6.11}$$

V is close to h but slightly larger, so both the exponentials' arguments are negative.

For large times we can discard the quickly-decaying second exponential, and be left with

$$\mathbb{P} = \left|\frac{1}{2}\left(1 + \frac{V}{h}\right)e^{-(V-h)t}\right|^2 \sim \left(1 + \frac{\Omega^2}{2V^2}\right)\exp\left(-t\frac{\Omega^2}{V}\right) \tag{3.6.12}$$

So, weird normalizations for small times aside, $\gamma_{\text{eff}} = \Omega^2/V$, but $\Omega = \tau^{-1}$, so $V = R$, the 'rate of observation': the stronger the coupling, the more the other system influences ours.

3.7 Non-unitary evolution

It happens when the particle can escape the system; for example in optical systems there can be a complex index of refraction. The Hamiltonian will look like

$$H = H_0 - iV\mathbb{1} \tag{3.7.1}$$

where $V \in \mathbb{R}^+$. The unitary evolution has an i multiplying the Hamiltonian, so we get a decreasing real exponential.

We will have $A \sim 1 - V\delta t + O(\delta t^2)$, so $\mathbb{P} \sim 1 - 2V\delta t + O(\delta t^2)$: the first derivative is nonzero!

An example of a nonhermitian Hamiltonian We consider a system and its environment together:

$$H = \underbrace{\Omega\sigma_x}_{\text{system}} + \underbrace{\int \mathrm{d}\omega\,|\omega\rangle\langle\omega|}_{\text{environment}} + \underbrace{\sqrt{\frac{\Gamma}{2\pi}}\int \mathrm{d}\omega\, g(\omega)(|-\rangle\langle\omega| + |\omega\rangle\langle -|)}_{\text{interaction}} \tag{3.7.2}$$

Where σ_x is meant to be in the $|-\rangle, |+\rangle$ basis. Now, let us take a generic state $|\psi\rangle = x(t)|-\rangle + y(t)|+\rangle + \int d\omega\, z(\omega,t)|\omega\rangle$.

We will write the Schrödinger equation for the evolution of x, y and z and show that, if we just consider the first two, the effective Hamiltonian looks like the one in (3.6.8).

The system so solve can be separated into

$$i\dot{x} = \Omega y \tag{3.7.3a}$$

$$i\dot{y} = \Omega x + \sqrt{\frac{\Gamma}{2\pi}} \int z\, d\omega \tag{3.7.3b}$$

$$i\dot{z} = \omega z + \sqrt{\frac{\Gamma}{2\pi}} y \tag{3.7.3c}$$

In can be readiliy verified that, with starting conditions $x = 1$, $y = z = 0$, we have

$$z(\omega,t) = -i\sqrt{\frac{\Gamma}{2\pi}} \int_0^t d\tau\, y(\tau) e^{-i\omega(t-\tau)} \tag{3.7.4}$$

so we substitute into the equation for y

$$i\dot{y} = \Omega x - i\frac{\Gamma}{2\pi} \int d\omega \int_0^t d\tau\, y(\tau) e^{-i\omega(t-\tau)} \tag{3.7.5}$$

but $\int d\omega\, e^{-i\omega(t-\tau)} = 2\pi\delta(t-\tau)$: so

$$i\dot{y} = \Omega x - i\Gamma y(t)/2 \tag{3.7.6}$$

The factor $1/2$ comes from the fact we integrated a δ on the *boundary* of the domain. We can combine the results into

$$i\frac{d}{dt}\begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 0 & \Omega \\ \Omega & -i\Gamma/2 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} \tag{3.7.7}$$

3.8 Implementation of quantum gates

We want to implement a NOT gate (σ_x): we use a spin-1/2 particle, and two magnetic fields described by a Hamiltonian

$$H = -\mu\Big(B_0\sigma_z + B_1\Big(\cos(\omega t)\sigma_x + \sin(\omega t)\sigma_y\Big)\Big) \tag{3.8.1}$$

So the zeroth field is fixed on z, while the other rotates around the z axis staying on the xy plane.

TODO

3.9 Density matrices

Say we have a generic observable $\hat{A} = \sum_i a_i |a_i\rangle\langle a_i|$, and our has a probability p_i of being in the state $|\psi_i\rangle$: of course we must have $\sum_i p_i = 1$. Then, we want to compute the expectation

value $\langle A \rangle$ in this "mixed" state: it will look like

$$\langle A \rangle = \sum_{i,k} p_i a_k \langle \psi_i | a_k \rangle \langle a_k | \psi_i \rangle \tag{3.9.1a}$$

$$= \sum_{i,j,k} p_i a_k \langle a_k | \left(\left| a_j \right\rangle \left\langle a_j \right| \right) | \psi_i \rangle \langle \psi_i | a_k \rangle \tag{3.9.1b}$$

$$= \sum_k \langle a_k | \left(\sum_j \underbrace{a_k}_{\substack{k \equiv j \text{ since it is} \\ \text{multiplied by } \delta_{jk}}} \left| a_j \right\rangle \left\langle a_j \right| \right) \left(\sum_i p_i \left| \psi_i \right\rangle \left\langle \psi_i \right| \right) | a_k \rangle \tag{3.9.1c}$$

$$= \operatorname{Tr}(A\rho) = \operatorname{Tr}(\rho A) \tag{3.9.1d}$$

So, we have defined

$$\rho \stackrel{\text{def}}{=} \sum_k p_k \left| \psi_k \right\rangle \left\langle \psi_k \right| \tag{3.9.2}$$

Properties

1. $\operatorname{Tr} \rho = 1$
2. $\rho = \rho^\dagger$
3. $\rho \geq 0$
4. $\operatorname{Tr} \rho^2 \leq 1$

These can be deduced from writing the matrix elements $\rho_{ij} = \langle i | \rho \left| j \right\rangle$ in an ON basis, or by noticing that ρ is a positively-weighted sum of projectors, each of which is self-adjoint.

The first one needs the components approach, I think: $\rho_{ii} = \sum_{ik} \left| \langle \psi_k | i \rangle \right|^2 = 1$ since they are the components in a basis of a normalized ket.

The last property can be seen by noticing that ρ is self-adjoint, so it has an orthonormal basis: then squaring it is easy, and all the coefficients are such that $p_i^2 \leq p_i$.

Time evolution of a density matrix How does ρ evolve? If we have U, we can write the evolution by linearity as

$$\rho(t) = \sum_k p_k U \left| \psi_k \right\rangle \left\langle \psi_k \right| U^\dagger = U \rho_0 U^\dagger \tag{3.9.3}$$

If instead we wish to look at the differential formulation, starting from $i\hbar \left| \dot{\psi}_k \right\rangle = H \left| \psi_k \right\rangle$ and its adjunct $-i\hbar \left\langle \dot{\psi}_k \right| = \left\langle \psi_k \right| H$ we get

$$\frac{\mathrm{d}}{\mathrm{d}t} \rho(t) = \sum_k p_k \frac{\mathrm{d}}{\mathrm{d}t} \left(\left| \psi_k \right\rangle \left\langle \psi_k \right| \right) = \frac{1}{i\hbar} \sum_k p_k \left(H \left| \psi_k \right\rangle \left\langle \psi_k \right| - \left| \psi_k \right\rangle \left\langle \psi_k \right| H \right) = \frac{[H, \rho]}{i\hbar} \tag{3.9.4}$$

Pure states A density matrix is a *pure state* if it has only one component, in the sense that: $\rho = |\psi\rangle\langle\psi|$. The following are equivalent:

1. ρ is a density matrix;
2. ρ has rank 1;
3. $\operatorname{Tr}\rho^2 = 1$.

The quantity $\operatorname{Tr}\rho^2$ is called the *purity*, and is surely greater than $1/d$, d being the dimension of the Hilbert space (consider $\rho = d^{-1}\mathbb{1}$).

Examples of density matrices For a single pure qubit:

$$\rho = |\psi\rangle\langle\psi| = \begin{bmatrix} \cos^2(\theta/2) & \cos(\theta/2)\sin(\theta/2)e^{-i\varphi} \\ \cos(\theta/2)\sin(\theta/2)e^{i\varphi} & \sin^2(\theta/2) \end{bmatrix} \tag{3.9.5}$$

For a generic one-qubit mixed state:

$$\rho = \frac{1}{2}(\mathbb{1} + \vec{r}\cdot\vec{\sigma}) = \frac{1}{2}\begin{bmatrix} 1 \\ x \\ y \\ z \end{bmatrix} \cdot \begin{bmatrix} \mathbb{1} \\ \sigma_x \\ \sigma_y \\ \sigma_z \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 1+z & x-iy \\ x+iy & 1-z \end{bmatrix} \tag{3.9.6}$$

it can be shown by direct computation that in this case $\operatorname{Tr}\rho^2 = 1/2(1+|r|^2)$,where $\vec{r} = (x,y,z)$: so the state is pure for $|\vec{r}| = 1$, and the purity is quadratic in $|\vec{r}|$.

We could also look at $\det\rho = 1/4(1-|r|^2)$ and see that it is zero when $|\vec{r}| = 1$, but that method seems less powerful...

Composite systems Say we have two Hilbert spaces 1 and 2, with their respective orthonormal bases $|i\rangle$ and $|\alpha\rangle$ respectively (let us work with finite-dimensional ones for simplicity).

Say we want to calculate the expectation value of an observable A_1 on 1: we must write it as $A_T = A \otimes \mathbb{1}_2$. Of course, our density matrix will also have four indices. Then

$$\langle A\rangle = \operatorname{Tr}\left(\rho A_T\right) = \sum_{k\gamma}\langle k\gamma|\left(\sum_{ij\alpha\beta}\rho_{i\alpha}^{j\beta}|i\alpha\rangle\langle j\beta|\right)\left(\sum_{mn\sigma\xi}A_m^n\delta_\sigma^\xi|m\sigma\rangle\langle n\xi|\right)|k\gamma\rangle \tag{3.9.7}$$

So we can make the sums implicit, the components of A explicit, and simplify some δs:

$$\operatorname{Tr}\left(\rho A_T\right) = \delta_k^i\delta_\gamma^\alpha\rho_{i\alpha}^{j\beta}\delta_j^m\delta_\beta^\sigma A_m^n\delta_\sigma^\xi\delta_n^k\delta_\xi^\gamma = \rho_{i\alpha}^{j\alpha}A_j^i \tag{3.9.8}$$

The simplifications are easier to understand by writing the index equivalencies: $m \equiv j$, $i \equiv k \equiv n$ and $\alpha \equiv \gamma \equiv \xi \equiv \sigma \equiv \beta$.

The trace with a simple one-subsystem density matrix, with the same one-subsystem observable A, would look like

$$\operatorname{Tr}\left(\rho A\right) = \rho_i^j A_j^k\delta_k^i = \rho_i^j A_j^i \tag{3.9.9}$$

So it becomes clear that we can use the traced matrix $\rho_{i\alpha}^{j\alpha} \overset{\text{def}}{=} (\rho_1)_i^j$ as a *reduced density matrix* for the first subsystem.

We can write this in index-free notation as

$$\rho_1 = \operatorname*{Tr}_2 \rho \tag{3.9.10}$$

Note that even when ρ is a pure state, if we trace out a subsystem it can become mixed: this can be seen with $\rho = 1/2(|00\rangle + |11\rangle)(\langle 00| + \langle 11|)$, whose $\rho_1 = 1/2(|0\rangle\langle 0| + |1\rangle\langle 1|)$.

3.10 Correlations

We want to characterize quantum observables x and y. Let us start by defining the standard deviation:

$$\sigma_x = \sqrt{\left\langle (x - \langle x \rangle)^2 \right\rangle} \tag{3.10.1}$$

So, we can define the covariance between two variables:

$$C_{xy} = \frac{\left\langle (x - \langle x \rangle)(y - \langle y \rangle) \right\rangle}{\sigma_x \sigma_y} = \frac{\langle xy \rangle - \langle x \rangle \langle y \rangle}{\sigma_x \sigma_y} \tag{3.10.2}$$

(Unless $[x, y] = 0$ this is not the same as C_{yx}!)

3.11 Schmidt decomposition

Let us take a generic state in a two-subsystem system: $|\psi\rangle = \sum_{i,\alpha} c_{i\alpha} |i\rangle_A |\alpha\rangle_B$. In general, this will be a superposition of $\dim A \dim B$ states. Schimdt says we can write it as

$$|\psi\rangle = \sum_{i=1}^{k} \sqrt{p_i} |i\rangle_A |\alpha(i)\rangle_B \tag{3.11.1}$$

where k is called the *Schmidt rank*, and the $|\alpha(i)\rangle$ are orthormal. Also, $p_i \geq 0$ and $\sum_i p_i = 1$. How do we get this? We start from our generic state and rewrite it:

$$\begin{aligned} |\psi\rangle &= \sum_{i,\alpha} c_{i\alpha} |i\rangle_A |\alpha\rangle_B && \text{(3.11.2a)} \\ &= \sum_i |i\rangle \left(\sum_\alpha c_{i\alpha} |\alpha\rangle \right) && \text{(3.11.2b)} \\ &= \sum_i |i\rangle |\widetilde{\alpha}(i)\rangle && \text{(3.11.2c)} \end{aligned}$$

This seems fine, but the $|\widetilde{\alpha}(i)\rangle$ do not have the properties we want: they are not orthonormal. Let us use equation (3.9.10), with an explicit one-subsystem matrix, and set it equal to the density matrix of (3.11.2c).

$$\sum_i p_i |i\rangle\langle i| = \operatorname*{Tr}_2 \left(\sum_{i,j} |i\rangle |\widetilde{\alpha}(i)\rangle \langle j| \langle \widetilde{\alpha}(j)| \right) \tag{3.11.3a}$$

$$= \sum_\gamma \langle\gamma| \left(\sum_{i,j} |i\rangle \left|\widetilde{\alpha}(i)\right\rangle \langle j| \left\langle\widetilde{\alpha}(j)\right| \right) |\gamma\rangle \tag{3.11.3b}$$

$$= \sum_{i,j} |i\rangle \langle j| \left(\left\langle\widetilde{\alpha}(i)\right| \left(\sum_\gamma |\gamma\rangle\langle\gamma| \right) \left|\widetilde{\alpha}(j)\right\rangle \right)^* \tag{3.11.3c}$$

$$= \sum_{i,j} |i\rangle \langle j| \left\langle\widetilde{\alpha}(j)\middle|\widetilde{\alpha}(i)\right\rangle \tag{3.11.3d}$$

So, in order for the equality to work it must be that $\left\langle\widetilde{\alpha}(j)\middle|\widetilde{\alpha}(i)\right\rangle = p_i\delta_{ij}$. So, we can rewrite equation (3.11.2c) with $\left|\widetilde{\alpha}(i)\right\rangle \to \left|\widetilde{\alpha}(i)\right\rangle / \sqrt{p_i}$, which are orthonormal. So, we get

$$|\psi\rangle = \sum_i \sqrt{p_i} |i\rangle \left|\widetilde{\alpha}(i)\right\rangle \tag{3.11.4}$$

and the properties of the p_i are inherited from the one-subsystem matrix.
Note that the Schmidt rank is very susceptible to small perturbations.

Correletions for separable states A separable state can be written as $|\psi\rangle = |i\rangle_A |\alpha\rangle_B$. If we have an observable on either system, then the correlation will be zero, since the averaging in $\langle x_A y_B\rangle$ will factor.

Purification If we have a generic state $\rho = \sum_i p_i |i\rangle\langle i|$, we can add a second subsystem in order to make it into a pure state: let us call the full density matrix $\sigma = |\psi\rangle\langle\psi|$, which must equal ρ if we trace out the second system. The components of σ will look like $\sigma_{i\alpha}^{j\beta} = c_{i\alpha}c_{j\beta}^*$, c being the components of $|\psi\rangle$ in the two-system basis.

$$\rho = \sum_\gamma \langle\gamma| \left(\sum_{ij\alpha\beta} \sigma_{i\alpha}^{j\beta} |i\alpha\rangle \langle j\beta| \right) |\gamma\rangle \tag{3.11.5a}$$

$$= \sum_{ij\alpha\beta} \sigma_{i\alpha}^{j\beta} |i\rangle \langle j| \langle\beta|\alpha\rangle \tag{3.11.5b}$$

$$\sum_{ij} \rho_{ij} |i\rangle\langle j| = \sum_{ij\alpha\beta} c_{i\alpha}c_{j\beta}^* \delta_\alpha^\beta |i\rangle\langle j| \tag{3.11.5c}$$

So the equation to be solved is $\rho_{ij} = c_{i\alpha}c_{j\alpha}^*$: these are $(\dim A)^2$ equations, and we have $(\dim B)^2$ parameters to tweak: so this can always be done with $\dim B = \dim A$.

3.12 Kraus representation

How does a subsystem ρ_1 of $\rho = \rho_1 \otimes |G\rangle\langle G|_2$ evolve? We are using a pure state for subsystem 2 but the construction will be general, since as we saw in 'Purification' on page 60 we can purify states. We know that $\rho(t) = U\rho U^\dagger$, so:

$$\rho_1(t) = \operatorname*{Tr}_2 \left(U(\rho_1 \otimes |G\rangle\langle G|_2) U^\dagger \right) = \sum_k \langle k| U |G\rangle \rho_1 \langle G| U^\dagger |k\rangle \tag{3.12.1}$$

so we define $E_k = \langle k| U |G\rangle$. Note that this is still a matrix, since we only contracted the subsystem 2 indices. These matrices obey $\sum_k E_k^\dagger E_k = \mathbb{1}$. With this, we get

$$\rho_1(t) = \sum_k E_k \rho_1 E_k^\dagger \tag{3.12.2}$$

This defines a *superoperator* $\mathcal{S} : \rho \to \sum_k E_k \rho E_k^\dagger$.
Because of how it was defined, $\mathcal{S}$ has the following properties:

1. it preserves self-adjointness;
2. it preserves the trace;
3. it preserves non-negativity.

The set of the $\mathcal{S}$ also has a group structure, and $\mathcal{S}^{-1}$ exists iff $\mathcal{S}$ is unitary.

Kraus representations Any superoperator with properties 1, 2 and 3 it can be written as

$$\mathcal{S}(\rho) = \sum_k E_k \rho E_k^\dagger \tag{3.12.3}$$

3.13 Generalized measurements

A generalized measurement is defined by a set of operators M_i, such that $\sum_i M_i^\dagger M_i = \mathbb{1}$. They represent the possible results of the measurement: the wavefunction is reduced to

$$\frac{M_i |\psi\rangle}{\|M_i \psi\|} \qquad \text{with probability} \qquad p_i = \left\| M_i |\psi\rangle \right\|^2 = \langle\psi| M_i^\dagger M_i |\psi\rangle \tag{3.13.1}$$

Note that the probabilities are normalized: $\sum_i p_i = 1$.
If all the M_i are projectors ($M_i = M_i^\dagger = M_i^2$) then we get the usual Von Neumann projective measurements.

Naimark Theorem Generalized measurements are equivalent to projective measurements in a larger space: more specifically, a generalized measurement is equivalent to:

1. Adding some ancillary qubits;
2. evolving the whole system unitarily;
3. taking a projective measurement.

Unitary characterization of Kraus evolution We have some Kraus evolution $\rho \to \sum_k E_k \rho E_k^\dagger$, with $\sum_k E_k^\dagger E_k = \mathbb{1}$.
Let us introduce a subsystem 2, with dimension the number of Kraus operators, and its orthonormal basis $|k\rangle$, and the operator

$$U |\psi\rangle_1 |0\rangle_2 \stackrel{\text{def}}{=} \sum_k E_k |\psi\rangle_1 |k\rangle_2 \tag{3.13.2}$$

Claim 3.13.1. *U as defined is unitary.*

Proof. We can show this by proving $\langle \psi 0 | U^\dagger U | \psi 0 \rangle = 1$. This is then just a calculation:

$$\langle \psi 0 | U^\dagger U | \psi 0 \rangle = \sum_{k,k'} \langle \psi |_1 \langle k' |_2 E_{k'} E_k | \psi \rangle_1 | k \rangle_2 = \langle \psi |_1 \left(\sum_k E_k^\dagger E_k \right) | \psi \rangle_2 = 1 \tag{3.13.3}$$

□

Claim 3.13.2. *Taking the Kraus evolution of $\rho_1 = |\psi\rangle\langle\psi|$ is equivalent to evolving $\rho = |\psi 0\rangle\langle\psi 0|$ according to U and then tracing out subsystem 2.*

Proof. The evolution of ρ is $\sum_{k,m} E_k |\psi\rangle_1 |k\rangle_2 \langle\psi|_1 \langle m|_2 E_m^\dagger$. Let us take the trace of this wrt subsystem 2: we get

$$\sum_j \langle j |_2 \left(\sum_{k,m} E_k |\psi\rangle_1 |k\rangle_2 \langle\psi|_1 \langle m|_2 E_m^\dagger \right) |j\rangle_2 = \sum_k E_k |\psi\rangle\langle\psi|_1 E_k^\dagger = \sum_k E_k \rho_1 E_k^\dagger \tag{3.13.4}$$

□

Claim 3.13.3. *Evolving $|\psi\rangle |0\rangle$ according to U and then taking a projective measurement is equivalent to a generalized measurement on subsystem 1.*

Proof. We take the measurement $P = \mathbb{1}_1 \otimes |i\rangle\langle i|_2$.

$$\operatorname*{Tr}_{12}(\rho P_i) = \sum_{jq} \langle j |_1 \langle q |_2 \left(\sum_{k,m} E_k |\psi\rangle_1 |k\rangle_2 \langle\psi|_1 \langle m|_2 E_m^\dagger \right) (\mathbb{1}_1 \otimes |i\rangle\langle i|_2) |j\rangle_1 |q\rangle_2 \tag{3.13.5a}$$

$$= \sum_j \langle j |_1 \left(E_i |\psi\rangle\langle\psi|_1 E_i^\dagger \right) |j\rangle_1 \tag{3.13.5b}$$

$$= \operatorname*{Tr}_1 \left(|\psi\rangle\langle\psi| E_i^\dagger E_i \right) \tag{3.13.5c}$$

□

Weak measurements We wish to measure a system without disturbing it too much: let us consider a System-Environment couple of qubits, in the initial state $|\psi\rangle = (\alpha |0\rangle + \beta |1\rangle)_S \otimes |0\rangle_E = \alpha |00\rangle + \beta |10\rangle$. We apply the gate

$$U = (R_z(\theta)_S \otimes \mathbb{1}_E)\big(\cos(\theta)\mathbb{1}_{SE} - i\sin(\theta)\mathrm{C_SNOT}_E\big) = \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & e^{i\theta}\cos\theta & -ie^{i\theta}\sin\theta \\ & & -ie^{i\theta}\sin\theta & e^{i\theta}\cos\theta \end{bmatrix} \tag{3.13.6}$$

(Why is the phase included?)

(θ is small). The result of the application of this gate to $|\psi\rangle$ is

$$U |\psi\rangle = \alpha |00\rangle + \beta e^{i\theta} \big(\cos(\theta) |10\rangle - i\sin(\theta) |11\rangle\big) \tag{3.13.7}$$

Now, we measure the environment: we will most likely (with probability $\sim 1 - |\beta|^2\theta^2$) get 0: in this case the system is reduced to

$$\frac{\alpha|00\rangle + \beta e^{i\theta}\cos(\theta)|10\rangle}{\sqrt{|\alpha|^2 + |\beta\cos(\theta)|^2}} \tag{3.13.8}$$

which approaches $|\psi\rangle$ as $\theta \to 0$. If, instead, we get 1, the state becomes $|11\rangle$.

This does not seem very useful, as it can only provide us with some statistical bounds on the size of β if we measure a few times, but we must not do it too often...

3.13.1 POVMs

We get some set of positive operators F_i such that $\sum_i F_i = \mathbb{1}$, and use these as the possible results of our measurement, which we will get with probabilities $p_i = \langle\psi|F_i|\psi\rangle$.

They are useful in describing destructive measurements, like a photodetector. It is interesting when $p_i = 0$ with some ψ, because if we see that detector go off we know the system was *not* in ψ.

3.14 Quantum channels

An example of decoherence by interaction If our first system starts in $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$, so

$$\rho = \begin{bmatrix} |\alpha|^2 & \alpha\beta^* \\ \alpha^*\beta & |\beta|^2 \end{bmatrix} \tag{3.14.1}$$

Now, let us consider a second subsystem, so the state becomes $\alpha|00\rangle + \beta|10\rangle$, then we apply a CNOT gate controlling on our first subsystem: the state becomes $\alpha|00\rangle + \beta|11\rangle$. If we trace the second subsystem out, the density matrix becomes

$$\rho' = \begin{bmatrix} |\alpha|^2 & 0 \\ 0 & |\beta|^2 \end{bmatrix} \tag{3.14.2}$$

Linear transformations in Bloch space We take a Kraus transformation of a density matrix as given in equation (3.12.3), and represent it as in equation (3.9.6): $\rho = 1/2(\mathbb{1} + \vec{r}\cdot\vec{\sigma})$ (and in the same fashion ρ' with r').

Claim 3.14.1. *This Kraus transformation corresponds to a linear map $r_i \to M_i^j r_j + c_i$ which is a contraction.*

Proof. We can expand the Kraus matrices as $E_k = \gamma_k\mathbb{1} + \sum_i a_{ik}\sigma_i$: our full expression becomes

$$\rho \to \rho' = \sum_k \left(\gamma_k\mathbb{1} + \sum_i a_{ik}\sigma_i\right)\frac{1}{2}(\mathbb{1} + \vec{r}\cdot\vec{\sigma})\left(\gamma_k^*\mathbb{1} + \sum_j a_{jk}^*\sigma_j^\dagger\right) \tag{3.14.3}$$

and our claim is that

$$\rho' = \frac{1}{2}\left(\mathbb{1} + \left(M_i^j r_j + c_i\right)\sigma_i\right) \tag{3.14.4}$$

for some matrix M_i^j and vector c_i. This can be readily seen by noticing that:

1. products of Pauli matrices are linear combinations of Pauli matrices: $\sigma_a\sigma_b = \delta_{ab}\mathbb{1} + i\varepsilon_{abc}\sigma_c$;
2. the Kraus transformation sends density matrices into density matrices, so the trace of ρ' will still be 1 and we will be able to separate the trace term $\mathbb{1}/2$ from the traceless Pauli matrix part (that is, there will not be any transformation-dependents coefficients multiplying the identity).

Now, to see that it is a contraction recall that $\operatorname{Tr}\rho^2 \leq 1$. We will apply the formula:

$$(\vec{a}\cdot\vec{\sigma})(\vec{b}\cdot\vec{\sigma}) = (\vec{a}\cdot\vec{b})\mathbb{1} + i(\vec{a}\wedge\vec{b})\cdot\vec{\sigma}) \tag{3.14.5}$$

So then:

$$\operatorname{Tr}(\rho')^2 = \operatorname{Tr}\left(\frac{1}{4}\left(\mathbb{1}+\vec{r'}\cdot\vec{\sigma}\right)^2\right) = \operatorname{Tr}\left(\frac{1}{2}\left(\frac{1+\left|r'\right|^2}{2}\mathbb{1}+\vec{r'}\cdot\vec{\sigma}\right)\right) \tag{3.14.6}$$

therefore $\left|r'\right| \leq 1$: the image of the unit sphere is contained in the unit sphere. □

We can write explicit expressions for M and c:

$$M_{jk} = \sum_l \left(2\operatorname{Re}\left(a_{lj}a_{lk}^*\right) + \delta_{jk}\left(\left|\gamma_l\right|^2 - \sum_p \left|a_{lp}\right|^2\right) + 2\sum_p \varepsilon_{jkp}\operatorname{Im}\left(\gamma_l^* a_{lp}\right)\right) \tag{3.14.7a}$$

$$c_j = 2i\sum_{klm}\varepsilon_{jlm}a_{kl}a_{km}^* \tag{3.14.7b}$$

It seems like it should be true that $|\det M| = 1$ (and $\vec{c} = 0$) iff there is only one E_k, that is, the channel is actually a unitary transformation.

***-flip channel**

$$\mathcal{S}(\rho) = |\alpha|^2\sigma_i\rho\sigma_i^\dagger + \left(1-|\alpha|^2\right)\rho \tag{3.14.8}$$

So $E_0 = \alpha\sigma_i$ and $E_1 = \sqrt{1-|\alpha|^2}\mathbb{1}$.

1. $i = x$: bitflip
2. $i = z$: phaseflip
3. $i = y$: bitphaseflip

In the Bloch sphere, it keeps the dimension i still and shrinks along the other two by a factor $1-2|\alpha|^2$. For example, the bitflip gate approaches σ_x as $|\alpha|^2 \to 1$.

This circuit can be represented as unitary evolution: we add a subsystem with a wavefunction $|\psi\rangle = \alpha|1\rangle + \sqrt{1-|\alpha|^2}|0\rangle$, and perform a control-$\sigma_i$ (where the new subsystem is the controller).

In the expression of ψ the 0 and 1 are swapped, right?

Depolarizing channel It mixes states: the fixed point is $r = 0$.

$$\mathcal{S}(\rho) = \frac{P}{3}\left(\sum_i \sigma_i \rho \sigma_i^\dagger\right) + (1-P)\rho \tag{3.14.9}$$

$$r \to r\left(1 - \frac{4P}{3}\right) \tag{3.14.10}$$

Amplitude damping channel Its Kraus matrices are

$$E_0 = \begin{bmatrix} 1 & 0 \\ 0 & \sqrt{1-P} \end{bmatrix} \qquad E_1 = \begin{bmatrix} 0 & \sqrt{P} \\ 0 & 0 \end{bmatrix} \tag{3.14.11}$$

It moves the population towards $|0\rangle\langle 0|$: it maps $|1\rangle\langle 1| \to P\,|0\rangle\langle 0| + (1-P)\,|1\rangle\langle 1|$.

The fixed point is a pure state, so this channel can increase the purity of a state; however, it is fundamentally an incoherent process.

In the Bloch sphere, the amplitude damping channel looks like:

$$r \to \begin{bmatrix} \sqrt{1-P} & & \\ & \sqrt{1-P} & \\ & & 1-P \end{bmatrix} r + \begin{bmatrix} 0 \\ 0 \\ P \end{bmatrix} \tag{3.14.12}$$

So, for example, $r = -\hat{z} \to (2P-1)\hat{z}$. This transformation has only $(0,0,1)^\top$ as its fixed point.

Phase damping channel It models what we might see if our particle was in a variable magnetic field: the phase of the particle is rotated by varying similar continuously distributed angles. We can write the phase gate as $R_z(\theta) = \operatorname{diag}\left(e^{-i\theta/2}, e^{i\theta/2}\right)$. We assume the phase angles are normally distributed with variance λ:

$$p(\theta) = \frac{\exp\left(\frac{-\theta^2}{2\lambda}\right)}{\sqrt{\pi\lambda}} \tag{3.14.13}$$

then the channel looks like

$$\rho \to \int_{-\infty}^{+\infty} R_z(\theta)\rho R_z(-\theta) p(\theta)\,\mathrm{d}\theta \tag{3.14.14}$$

Now let us take a generic density matrix:

$$\rho = \begin{bmatrix} P & \alpha \\ \alpha^* & 1-P \end{bmatrix} \to \int \mathrm{d}\theta\, p(\theta) \begin{bmatrix} P & \alpha e^{-i\theta} \\ \alpha^* e^{i\theta} & 1-P \end{bmatrix} \tag{3.14.15}$$

and by putting together $p(\theta)e^{\pm i\theta}$ we can complete the square to get a Gaussian integral (which equals one since the pdf is already normalized) times $e^{-\lambda}$. So

$$\rho' = \begin{bmatrix} P & \alpha e^{-\lambda} \\ \alpha^* e^{-\lambda} & 1-P \end{bmatrix} \tag{3.14.16}$$

This can be also be interpreted as repeated application of the channel with the Kraus matrices

$$E_0 = \sqrt{1-P}\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix} \qquad E_2 = \sqrt{P}\begin{bmatrix}0 & 0\\ 0 & 1\end{bmatrix} \qquad E_2 = \sqrt{P}\begin{bmatrix}1 & 0\\ 0 & 0\end{bmatrix} \tag{3.14.17}$$

which send

$$\rho \to \begin{bmatrix}\rho_{00} & \rho_{01}(1-P)\\ \rho_{10}(1-P) & \rho_{11}\end{bmatrix} \tag{3.14.18}$$

and if $P = \lambda\delta t$ for small δt and the interactions are very fast then $\rho'_{01} \to (1-\lambda\delta t)^{t/\delta t} \sim e^{-\lambda t}$.

Entanglement damping channel Let us consider a nice entangled couple of qubits, with $|\psi\rangle = 1/\sqrt{2}(|01\rangle + |10\rangle)$. How can we break it? We will use the Kraus operators $E_{1,2} = \mathbb{1} \otimes \mathrm{diag}\big(1, \cos(\theta)\big)$ or $\mathbb{1} \otimes \mathrm{diag}\big(1, \sin(\theta)\big)$.

Then, the density matrix becomes:

$$\frac{1}{2}\begin{bmatrix}1 & 1\\ 1 & 1\end{bmatrix} \to \frac{1}{2}\begin{bmatrix}1 & \cos(\theta)\\ \cos(\theta) & 1\end{bmatrix} \tag{3.14.19}$$

If we trace out one subsystem, we get $\rho_i = 1/2\mathbb{1}$, before and after the transformation.

3.15 Master equation

We want to describe the time evolution of a system with Kraus matrices:

$$\rho(t) = \mathcal{S}(t, t_0)[\rho] = \sum_{k=0}^{N-1} E_k \rho E_k^\dagger \tag{3.15.1}$$

with $N \leq (\dim\mathcal{H})^2$. It must have the following properties:

1. $\mathcal{S}(t,t) = \mathbb{1}$;
2. It should become the conventional unitary evolution if $N = 1$;
3. at any time, we must have $\sum_k E_k^\dagger E_k = \mathbb{1}$.

How will these matrices look? We would like to assume $E_0 = \mathbb{1} + H/i\hbar\,\mathrm{d}t$, but this will not work: let us add a term $K\,\mathrm{d}t$, with a self-adjoint K.

The other E_k will then be $L_k\sqrt{\mathrm{d}t}$ to first order.

Expanding condition 3 to first order gives:

$$\left(\left(\mathbb{1} + \left(\frac{H}{i\hbar} + \frac{K}{\hbar}\right)\mathrm{d}t\right)\left(\mathbb{1} + \left(-\frac{H}{i\hbar} + \frac{K}{\hbar}\right)\mathrm{d}t\right) + \sum_k L_k^\dagger L_k\right)\mathrm{d}t \stackrel{!}{=} \mathbb{1}\,\mathrm{d}t \tag{3.15.2}$$

So, we must have $K = -\hbar/2\sum_k L_k^\dagger L_k$ (indeed self-adjoint). How will our density matrix evolve after $\mathrm{d}t$ then? We will assume $\mathcal{S}(t+\mathrm{d}t\,, t)[\rho] = \rho + \dot\rho\,\mathrm{d}t + O(\mathrm{d}t^2)$.

$$\dot{\rho} = \frac{[H,\rho]}{i\hbar} + \frac{\{K,\rho\}}{\hbar} + \sum_k L_k \rho L_k^\dagger \tag{3.15.3}$$

We can plug in our formula for K and compact the sums into one, to get the

Gorini–Kossakowski–Sudarshan–Lindblad equation

$$\dot{\rho} = \frac{[H,\rho]}{i\hbar} + \sum_k \left(L_k \rho L_k^\dagger - \frac{1}{2}\left\{ L_k^\dagger L_k, \rho \right\} \right) \tag{3.15.4}$$

This works if the system has no memory. If, instead, the evolution depends not only on the present state but on events further past, we must use the

Markovian version The form we show here is the diagonal one. We have the restriction that the L_k must be traceless.

$$\dot{\rho} = \frac{[H,\rho]}{i\hbar} + \sum_k \gamma_k \left(L_k \rho L_k^\dagger - \frac{1}{2}\left\{ L_k^\dagger L_k, \rho \right\} \right) \tag{3.15.5}$$

3.16 One-key cryptography

The simplest paradigm: we have a key k, decryption and encryption algorithms D and E: if P is the clear-text message and C is the encrypted one then $E_k(P) = C$ and $D_k(C) = P$.

Even a very simple algorithm is secure if the key is longer than the message, private and only used once: for example, if we have n letters in our alphabet, we can do $E_k P_i = (P_i - k_i) \mod n$ and $E_k C_i = (C_i + k_i) \mod n$.

We can distribute the keys with *Quantum Key Distribution*: there are different algorythms to do it, a modern one we will not treat uses entanglement and is called E91 since Eckert invented it. We will look at Bennet & Brassard.

Quantum Key Distribution: BB84 Alice wants to send Bob a secure string of ones and zeroes.

She selects two bases, say $B_z = \{|0\rangle, |1\rangle\}$ and $B_x = \{H|0\rangle, H|1\rangle\}$ (where we use the Hadamard gate, see 'Hadamard' on page 49).

At random, she chooses a basis with which to send each qubit, and keeps a record of the bases she used.

Bob receives the qubits and also measures them in a basis chosen between B_z and B_x, and keeps a record of the bases he used.

After the communication is finished, they exchange in clear text the list of the bases they used, and discard the bits where they used a different basis.

Now they have a secure shared list of bits: if Eve were to try to measure the qubits in the middle, around half the time she'd collapse the state into the wrong basis. So, Alice and Bob just need to check a portion of the bits they *should* share, and if they don't match then something is wrong: either there is too much noise, or somebody's listening in. Either way, they discard the whole key and try again.

Correction methods

1. First of all, we check on a part of our message the error rate R: if R/N is large ($\sim 1/2$) then we discard everything.
2. Now that we know R, we can choose some length ℓ such that $R\ell/N$ is still small: then, we do a parity check on every ℓ long block.
3. If we somehow know that Eve knows k bits of our message, we can still generate a key she will not be able to know: if we split our message into $n-k-s$ snippets for some s, she will be able to gather only $O(2^{-s})$ bits of information: after splitting the message, our *new* message is something like the parity of each snippet.

Attack methods Eve cannot intercept the qubits and resend them, that's the point. There are some things she could do, though:

1. **translucent attack**: Eve operates unitarily on the passing qubits, entangling them with some qubits she keeps, and which she measures only *after* Alice and Bob have communicated which basis they used.
   Surely she cannot completely *clone* the passing qubit, but she might do some sneaky low-interference stuff.
2. **collective attacks** on several qubits at once.

3.17 Dense coding

Bob and Alice prepare two qubits together, in $|\psi\rangle = \mathrm{CNOT}(H\otimes\mathbb{1})\,|00\rangle = {}^1/\sqrt{2}(|00\rangle + |11\rangle)$. Now Alice takes a qubit with her, and Bob keeps the other.

Now they are far apart. Alice wants to send two classical bits xy. She chooses based on her two bits an operator between $U_i = \left\{\mathbb{1}, \sigma_x, \sigma_z, \sigma_y\right\}$ and applies it to her qubit.

The state becomes one of these:

$$U_0\,|\psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \tag{3.17.1a}$$

$$U_1\,|\psi\rangle = \frac{1}{\sqrt{2}}(|10\rangle + |01\rangle) \tag{3.17.1b}$$

$$U_2\,|\psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle) \tag{3.17.1c}$$

$$U_3\,|\psi\rangle = \frac{1}{\sqrt{2}}(|10\rangle - |01\rangle) \tag{3.17.1d}$$

Now she sends her qubit to Bob, who still has his.

Bob applies $\big(\mathrm{CNOT}(H\otimes\mathbb{1})\big)^{-1}$ to the qubits.

$$\big(\mathrm{CNOT}(H\otimes\mathbb{1})\big)^{-1} = \begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & -1 \\ 0 & 1 & -1 & 0 \end{bmatrix} \tag{3.17.2}$$

Now, as can be seen by summing the combinations of rows of the matrix in (3.17.2) corresponding to the states $U_i\,|\psi\rangle$, Bob's qubits will be in the state $|xy\rangle$.

If we tried to do this with a mixed state, $\mathbb{1}$ and σ_z would give the same result ($1/2(|00\rangle\langle 00| + |11\rangle\langle 11|)$) as would σ_x and σ_y ($1/2(|01\rangle\langle 01| + |10\rangle\langle 10|)$). So, since there would be only two distinguishable states, only 1 bit would be transmitted.

3.18 Bell Inequalities

Alice and Bob have some (entangled) state on their hands, and are separated by a space-like interval. Alice makes a measurement x and gets outcome a, Bob makes a measurement y and gets outcome b.

They repeat this several times, always with the same starting state. This whole experiment is then characterized by the function $\mathbb{P}(ab|xy)$. In general we will have correlations, so $\mathbb{P}(ab|xy) \neq \mathbb{P}(a|x)\mathbb{P}(b|y)$. If our theory is local, however, these cannot be explained by the transmission of information from Alice to Bob. Can we describe them by some local unknown (*hidden*) variable which determines the measurement *a priori*?

Claim 3.18.1. *The results of a Bell experiment which are predicted by quantum mechanics* cannot *be described by a hidden variable λ distributed according to some function $q(\lambda)$, with an expression in the form:*

$$\mathbb{P}(ab|xy) = \int q(\lambda)\mathbb{P}(a|x;\lambda)\mathbb{P}(b|y;\lambda)\,\mathrm{d}\lambda \tag{3.18.1}$$

Proof. We prove the statement by contradiction. How do we calculate a correlation under our hypothesis? To simplify, we assume $a, b \in \{+1, -1\}$ and $x, y \in \{0, 1\}$. I will use the (improper) notation $\mathrm{d}q = \mathrm{d}\lambda\, q(\lambda)$

$$\langle ab\rangle_{xy} = \sum_{ab} ab\mathbb{P}(ab|xy) = \int \mathrm{d}q \left(\sum_a a\mathbb{P}(a|x;\lambda)\right)\left(\sum_b b\mathbb{P}(b|y;\lambda)\right) \tag{3.18.2}$$

Therefore, $\langle ab\rangle_{xy} = \int \mathrm{d}q\, \langle a\rangle_{x,\lambda} \langle b\rangle_{y,\lambda}$. Subscripts, here, mean conditioning.

Hidden variable inequality (CHSH) Now, we consider the following quantity:

$$S = \langle ab\rangle_{00} + \langle ab\rangle_{01} + \langle ab\rangle_{10} - \langle ab\rangle_{11} \tag{3.18.3}$$

The minus sign is arbitrarily placed, it just matters that there is just one negative and three positive terms. We can show that $S \leq 2$: surely

$$S \leq \int \mathrm{d}q \left[\left|\langle b\rangle_{0,\lambda} + \langle b\rangle_{1,\lambda}\right| \sup \langle a\rangle_{0,\lambda} + \left|\langle b\rangle_{0,\lambda} - \langle b\rangle_{1,\lambda}\right| \sup \langle a\rangle_{1,\lambda}\right] \tag{3.18.4}$$

and, since the outcomes are ± 1, for any λ: $\langle a\rangle_{x,\lambda} \leq 1$ and $\langle b\rangle_{y,\lambda} \leq 1$, so

$$S \leq \int \mathrm{d}q \left[\left|\langle b\rangle_{0,\lambda} + \langle b\rangle_{1,\lambda}\right| + \left|\langle b\rangle_{0,\lambda} - \langle b\rangle_{1,\lambda}\right|\right] \tag{3.18.5}$$

WLOG we can assume $\langle b\rangle_{0,\lambda} \geq \langle b\rangle_{1,\lambda} \geq 0$. Therefore the integrand is bounded by $\langle b\rangle_{0,\lambda} + \langle b\rangle_{1,\lambda} + \langle b\rangle_{0,\lambda} - \langle b\rangle_{1,\lambda} = 2\langle b\rangle_{0,\lambda} \leq 2$.

The probability density of λ must be normalized: $\int \mathrm{d}q = 1$. So, the integrand is an upper bound for the integral, and we get $S \leq 2$.

(This can be generalized to $|S| \leq 2$).

Quantum CHSH violation We use as our observables the spin in different directions: if we have a vector $\vec{a}$, then $\hat{O}_a = \vec{a} \cdot \vec{\sigma}$. As our state we take the antisymmetric spin singlet, $|\psi\rangle = 1/\sqrt{2}(|01\rangle - |10\rangle)$. We want to show that the correlation expectation value $\langle O_a \otimes O_b \rangle_\psi$ is equal to $-a \cdot b$. We only need to compute the central four elements of the 4x4 matrix $O_a \otimes O_b$, which correspond to the 01 and 10 basis elements.

$$[O_a \otimes O_b]_{\text{reduced}} = \begin{bmatrix} -a_z b_z & (a_x + ia_y)(b_x - ib_y) \\ (a_x - ia_y)(b_x + ib_y) & -a_z b_z \end{bmatrix} \tag{3.18.6}$$

We compute the expectation value of the matrix in (3.18.6):

$$\langle O_a \otimes O_b \rangle_\psi = \frac{1}{2} \begin{bmatrix} 1 & -1 \end{bmatrix} \begin{bmatrix} -a_z b_z & (a_x + ia_y)(b_x - ib_y) \\ (a_x - ia_y)(b_x + ib_y) & -a_z b_z \end{bmatrix} \begin{bmatrix} 1 \\ -1 \end{bmatrix} \tag{3.18.7a}$$

$$= \frac{1}{2}\Big(-a_z b_z - (a_x + ia_y)(b_x - ib_y) - (a_x - ia_y)(b_x + ib_y) + (-a_z b_z)\Big) \tag{3.18.7b}$$

$$= -\vec{a} \cdot \vec{b} \tag{3.18.7c}$$

Now: we pick as our measurement with possible outcomes $0, 1$ two *pairs* of directions, and we call the result 0 if the spin is measured along the first, 1 if it measured along the second.

1. For $\vec{a}$, we call the result 0 if the spin direction is $\vec{a}_0 = \hat{x}$ and 1 if the spin direction is $\vec{a}_1 = \hat{y}$;
2. for $\vec{b}$, we call the result 0 if the spin direction is $\vec{b}_0 = -(\hat{x} + \hat{y})/\sqrt{2}$ and 1 if the spin direction is $\vec{b}_1 = -(\hat{x} + \hat{y})/\sqrt{2}$

So, we can compute S using equation (3.18.7c):

$$S = \langle ab \rangle_{00} + \langle ab \rangle_{01} + \langle ab \rangle_{10} - \langle ab \rangle_{11} = \frac{4}{\sqrt{2}} = 2\sqrt{2} > 2 \tag{3.18.8}$$

□

3.19 Nonlocal correlations

We want to define *probability spaces*. We will use the notation of section Bell Inequalities. If a, b can have $\Delta \in \mathbb{N}$ values, and there are $m \in \mathbb{N}$ possible measurements (x, y) we can make. Then, our correlations are a point $\mathbb{P}(ab|xy)$ in some subset $\mathcal{P}$ of $\mathbb{R}^{m^2\Delta^2}$, bounded by:

1. $\forall x, y, a, b : \mathbb{P}(ab|xy) \geq 0$;
2. $\forall x, y$:

$$\sum_{a=1}^{\Delta} \sum_{b=1}^{\Delta} \mathbb{P}(ab|xy) = 1 \tag{3.19.1}$$

Now, we define some subsets of this space.

No-Signaling The set is called NS. We impose a condition which means: *no matter what we do with a measurement, it will not affect the other*: $\forall x, x', y, y', a$

$$\sum_{b=1}^{\Delta} \mathbb{P}(ab|xy) = \sum_{b=1}^{\Delta} \mathbb{P}(ab|xy') \qquad \sum_{a=1}^{\Delta} \mathbb{P}(ab|xy) = \sum_{a=1}^{\Delta} \mathbb{P}(ab|x'y) \tag{3.19.2}$$

this implies $\mathbb{P}(a|x) = \mathbb{P}(a|xy) = \sum_b \mathbb{P}(ab|xy)$.

In the $\Delta = 2$ case, $a, b = \pm 1$ the No-Signaling conditions become

$$\mathbb{P}(ab|xy) = \frac{1 + a\langle A_x\rangle + b\left\langle B_y\right\rangle + ab\left\langle A_x B_y\right\rangle}{4} \geq 0 \tag{3.19.3}$$

so if A and B have zero average, $1 \pm \left\langle A_x B_y\right\rangle \geq 0$.
What?

Local correlations The set is called L. It is the set of correlations that can be written as in equation (3.18.1).

Quantum correlations The set is called Q.

If we have some operators $M_{a|x}$ and $M_{b|y}$ in their respective Hilbert spaces, such that for each conditioning they still form a POVM (see 'POVMs' on page 63), then Q is the set of the probabilities which can be expressed as

$$\mathbb{P}(ab|xy) = \mathrm{Tr}(\rho_{AB} M_{a|x} \otimes M_{b|y}) \tag{3.19.4}$$

This is in the context of nonprojective measurements, but as we saw in 'Purification' on page 60 states can be purified so that everything we do is unitary. In that context,

$$\mathbb{P}(ab|xy) = \left\langle \psi \middle| A_x \otimes B_y \middle| \psi \right\rangle \tag{3.19.5}$$

with some self-adjoint families of operators A_x and B_y.

It can be useful to have $A_x B_y$, a product of commuting observables $[A_x, B_y] = 0$ on the same space, instead of $A_x \otimes B_y$; these descriptions are surely equivalent in the finite-dimensional case, maybe the latter is more general in the infinite-dimensional one.

Shapes and inclusions Every one of these sets is of the same dimension, and it can be shown that NS, L are polytopes while Q's boundary is curved. Also, $L \subset Q \subset NS \subset \mathcal{P}$.

They are all bounded, convex, closed. The planes which separate them are in general called Bell Inequalities.

The $\Delta = 2, m = 2$ case We can have different linearly independent Ss, (S being the one defined in (3.18.3)). In 2D (a projection?) we have: L is a square ($|S_x| \leq 2$, $\left|S_y\right| \leq 2$), Q is a circle ($|S|^2 \leq 8$), NS is a square ($\left|S'_{x,y}\right| \leq 4$, with $S'_{x,y} = HS_{x,y}$ (H is the Hadamard gate)).

3.20 Entropy

A message is a sequence of characters from an alphabet. If the alphabet is $\mathcal{A} = \{a_i\}_i$ and each of the characters in the alphabet appears with probability p_i, we can define $\mathcal{A}$'s *entropy* as

$$H = -\sum_i p_i \log(p_i) \tag{3.20.1}$$

with the convention $0 \log 0 = 0$

Noiseless coding: Shannon's theorem Given a k-long message, asyntotycally as $k \to \infty$ there exists an encoding with which we can express each character of the message with H bits on average, or the whole message with kH bits.

If we take any encoding, it can only do as good as Shannon encoding, and no better (at least not *in general*).

Von Neumann entropy We can define the entropy of a mixed state ρ as

$$S_V = -\operatorname{Tr}(\rho \log \rho) \tag{3.20.2}$$

1. For pure states we have $S_V(|\psi\rangle\langle\psi|) = 0$;
2. S_V is invariant wrt unitary transformations;
3. $0 \leq S_V \leq \dim \mathcal{H}$.[2]

Quantum Noiseless coding: Schumacher's theorem If our alphabet is now made of pure states, the probability distribution of a message will be some hyper-density matrix, $\rho^{\otimes N}$.

Schumacher says: in the limit of infinite message length, we can always compress it with S_V bits per letter.

3.21 Entanglement measurements

We want a measurement $E(\rho)$ which satisfies:

1. If ρ is separable, then $E(\rho) = 0$;
2. $E(\rho) = E(U\rho U^\dagger)$;
3. If we have a set of operators $A_i \otimes B_i$, to which we associate probabilities $p_i = \operatorname{Tr}\left((A_i \otimes B_i)\rho(A_i \otimes B_i)^\dagger\right)$, and which can project the state into $\sigma_i = (A_i \otimes B_i)\rho(A_i \otimes B_i)^\dagger / p_i$, then
$$E(\rho) \geq \sum_i p_i E(\sigma_i) \tag{3.21.1}$$

[2] Since $\prod_{i=1}^N p_i^{-p_i} \leq N$.

This means: the entanglement is invariant under local Kraus evolution: the systems cannot become *more* entangled when evolving on their own.

NOT CLEAR HOW

4. If $\rho = \rho_A$ is a pure state then $E(\rho) = S_V(\rho_A)$.

Entanglement of formation We can define

$$E_F(\rho) = \min \sum_i p_i S_V(\rho_A^i) \tag{3.21.2}$$

where the minimum is to be taken over all the possible decompositions $\rho = \sum_i p_i \left|\psi_i\right\rangle\!\left\langle\psi_i\right|$ and $\rho_A^i = \mathrm{Tr}_B(\left|\psi_j\right\rangle\!\left\langle\psi_j\right|)$: so, we pick a decomposition, we trace out the second system and take the entropy.

Concurrence This only applies to two-qubit systems.

$$C(\rho) = \max(0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4) \tag{3.21.3}$$

Where the λ_i are eigenvalues of $\left(\rho\sigma_y^{\otimes 2}\right)^2$, taken in decreasing order.

3.22 Quantum algorithms

3.22.1 Oracle interrogation

We have an oracle function $f(x) : \{0,1\}^n \to \{0,1\}$ which is either *constant* (always gives the same result) or *balanced* (gives 0 for half of its inputs, and 1 for the other half).

With a classical computer, we'd need $\max(\lfloor n/2 \rfloor, 2)$ calls to the oracle in the worst case to be sure that it is one and not the other. With a quantum computer, we can do it in just one call.

Take $n = 1$ for simplicity.

Our unitary representation of an oracle must be invertible, so we take the input along:

$$U_f \left|x\right\rangle \left|y\right\rangle \to \left|x\right\rangle \left|f(x) \oplus y\right\rangle \tag{3.22.1}$$

where $\oplus$ is the XOR binary gate. y is generic, it could be set to zero but we want a general gate. The algorithm is

1. Start with $\left|xy\right\rangle = \left|01\right\rangle$;
2. apply $H \otimes H$;
3. apply U_f;
4. apply $H \otimes \mathbb{1}$;
5. measure the first qubit.

First of all: $(H \otimes H)\,|01\rangle = (|0\rangle + |1\rangle)(|0\rangle - |1\rangle)/2$. Now:

$$U_f\,|x\rangle \otimes \left(\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right) = (-)^{f(x)}\,|x\rangle \otimes \left(\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right) \tag{3.22.2}$$

So after the application of the oracle gate, the first qubit's state has become

$$\frac{1}{\sqrt{2}}\Big((-)^{f(0)}\,|0\rangle + (-)^{f(1)}\,|1\rangle\Big) \tag{3.22.3}$$

and if we apply a Hadamard to it, it becomes

$$\frac{1}{2}\left(\Big((-)^{f(0)} + (-)^{f(1)}\Big)\,|0\rangle\,\Big((-)^{f(0)} - (-)^{f(1)}\Big)\,|1\rangle\right) \tag{3.22.4}$$

therefore the state is *surely* $|\psi\rangle = [f(0) = f(1)]\,|0\rangle + [f(0) \neq f(1)]\,|1\rangle$.

***n*-qubit case** We do the same thing as before, only with n qubits: $|x\rangle = |0\rangle^{\otimes n}$ at the start, so after the Hadamards we get

$$H^{\otimes(n+1)}\,|x\rangle\,|y\rangle = \frac{1}{2^{(n+1)/2}}\sum_{x=0}^{2^n-1}|x\rangle_1\,(|0\rangle - |1\rangle)_2 \tag{3.22.5}$$

so after applying the oracle and another Hadamard we get

$$H\left(\frac{1}{2^{n/2}}\sum_{x=0}^{2^n-1}(-)^{f(x)}\,|x\rangle\right) \tag{3.22.6}$$

on the first qubit. Now, either $f(x)$ is constant or it is balanced: if it is constant then this is just $|0\rangle$. If it is not, then it is orthogonal (since at least one of the bits must be different): so we can just check whether the system is in $|0\rangle$.

3.22.2 Grover

The classical complexity for a search in an unstructured database is $O(N)$, with Grover's algorithm we get $O(N^{1/2})$.

The problem looks similar to the oracle: now our $f(x) = [x = \overline{x}]$ and we seek $\overline{x}$. We explain the procedure with $n = 2$:

1. Start with $|xy\rangle = \left|\vec{0}1\right\rangle$;
2. apply $H^{\otimes(n+1)}$;
3. apply U_f;
4. apply $D \otimes \mathbb{1}$;
5. measure the $|x\rangle$ state.

as before, after applying step 3 we get

$$|\psi\rangle_1 = \frac{1}{2^{n/2}}\sum_{x=0}^{2^n-1}(-)^{f(x)}\,|x\rangle = \frac{1}{2^{n/2}}\left(\sum_{x=0}^{2^n-1}|x\rangle\right) - 2\,|\overline{x}\rangle \tag{3.22.7}$$

Now, D is $1/2$ of the matrix with -1 on the diagonal, and 1 in every other entry. Its eigenvectors are exactly the possible $|x\rangle$ after the oracle, so after the application of D we get exactly $|\overline{x}\rangle$.

This D can be made with the usual gates as $H^{\otimes 2}\sigma_x^{\otimes 2}(\mathbb{1}\otimes H)\mathrm{CNOT}(\mathbb{1}\otimes H)\sigma_x^{\otimes 2}H^{\otimes 2}$. Below is the Python code to verify that it works.

We will also need the matrix D', which is such that $D = H^{\otimes 2}D'H^{\otimes 2}$. It turns out that $D' = \eta_{\mu\nu}$ for a Minkowski flat spacetime.

```
import numpy as np
H = 1/np.sqrt(2)* np.array([[1,1], [1,-1]])
H2 = np.kron(H, H)
sigma_x = np.array([[0,1], [1,0]])
sigma_x2 = np.kron(sigma_x, sigma_x)
CNOT = np.array([[1,0,0,0],[0,1,0,0],[0,0,0,1],[0,0,1,0]])
idH = np.kron(np.identity(2), H)
print('D = ', H2 @ sigma_x2 @ idH @ CNOT @ idH @ sigma_x2 @ H2)
print('Dprime = ', sigma_x2 @ idH @ CNOT @ idH @ sigma_x2)
```

Arbitrary n This method only works for $n = 2$. In general, we have a state proportional $\sum_{x=0}^{2^n-1}|x\rangle|y\rangle$, an oracle such that $U_f|\overline{x}\rangle|y\rangle = -|\overline{x}\rangle|y\rangle$ while $U_f|x\rangle|y\rangle = |x\rangle|y\rangle$ for all the other $x \neq \overline{x}$.

Now, we can write $D' = \mathbb{1} - 2|0\rangle\langle 0|_1$: so $D = \mathbb{1} - 2|S\rangle\langle S|_1$, with $S = H^{\otimes 2}|0\rangle = \sum_{x=0}^{2^n-1}|x\rangle$.

Our main gate will be $G = DU_f$. What does it do? first, it flips the component of the state along $|\overline{x}\rangle$; then it flips the component along $|S\rangle$.

We know for sure that $|S\rangle$ and $|\overline{x}\rangle$ are not orthogonal: the angle between them will have $\cos(\varphi) = 2^{-n/2}$, the coefficient of $|\overline{x}\rangle$ in $|S\rangle$. We are interested in $\pi/2 - \varphi$, which we will call $\delta\theta$.

It can be shown by a simple geometric argument that the application of G sends a state which has an angle θ from the hyperplane $|\overline{x}\rangle^{\perp}$ into a state with an angle $\theta + 2\delta\theta$. So, we need K applications of G to get $\theta \to \pi/2$, with $K = (\pi/2)/(2\delta\theta)$: since $\sin\delta\theta = 2^{-n/2}$ and the rest are constants, $K = O(\sqrt{2^n}) = O(\sqrt{N})$, where N is the database size.

3.22.3 Quantum Fourier Transform

We have n qubits, and their states are $|x\rangle$ with x ranging from 0 to $N-1$, with $N = 2^n$.

Classical FFT The definition of the discrete Fourier transform of a vector x_i, with $i = 0, \ldots, N-1$, $(N = 2^n)$ is

$$X_k = \sum_{j=0}^{N-1} x_j \exp\left(-\frac{2\pi i j k}{N}\right) \tag{3.22.8}$$

To do this in $O(N\log N)$ instead of $O(N^2)$, we split the sum into the even and odd parts:

$$X_k = \sum_{j=0}^{N/2-1} x_{2j}\exp\left(-\frac{2\pi i(2j)k}{N}\right) + \exp\left(-\frac{2\pi i k}{N}\right)\sum_{j=0}^{N/2-1} x_{2j+1}\exp\left(-\frac{2\pi i(2j)k}{N}\right) \tag{3.22.9}$$

Or in other words

$$\mathrm{FFT}(x)_k = \mathrm{FFT}(\mathrm{even}(x))_k + \exp\left(-\frac{2\pi i k}{N}\right)\mathrm{FFT}(\mathrm{odd}(x))_k \tag{3.22.10}$$

Then, we can apply the same split for the FFT of the even and odd parts, and so on.

This split will happen $\log N = n$ times, after which there will just be one term in the sum. We have to to this computation once for every possible value of the result vector, so in the end the complexity is $O(N \log N)$.

Quantum version We define

$$\mathrm{QFT}(|J\rangle) = \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} \exp\left(\frac{2\pi i J k}{N}\right) |k\rangle \tag{3.22.11}$$

where as usual $|k\rangle = |k_0 k_1 \dots k_{n-1}\rangle$. So, we can rewrite this as a sum over all the k_α:

$$\begin{aligned}
\mathrm{QFT}(|J\rangle) &= \frac{1}{\sqrt{N}} \prod_{\alpha=0}^{n-1} \sum_{k_\alpha=0}^{1} \exp\left(-\frac{2\pi i J}{N}\right) \exp\left(\sum_{\alpha=0}^{n-1} k_\alpha 2^{n-\alpha-1}\right) |k\rangle && \text{(3.22.12a)} \\
&= \frac{1}{\sqrt{N}} \prod_{\alpha=0}^{n-1} \sum_{k_\alpha=0}^{1} \exp(-2\pi i J) \exp\left(\sum_{\alpha=0}^{n-1} k_\alpha 2^{-\alpha-1}\right) |k\rangle && \text{(3.22.12b)} \\
&= \frac{1}{\sqrt{N}} \prod_{\alpha=0}^{n-1} \sum_{k_\alpha=0}^{1} \exp\left(-2\pi i J k_\alpha 2^{-\alpha-1}\right) |k\rangle && \text{(3.22.12c)} \\
&= \frac{1}{\sqrt{N}} \prod_{\alpha=0}^{n-1} \left(\sum_{k_\alpha=0}^{1} \exp\left(-2\pi i J k_\alpha 2^{-\alpha-1}\right) |k_\alpha\rangle\right) && \text{(3.22.12d)} \\
&= \frac{1}{\sqrt{N}} \prod_{\alpha=0}^{n-1} \left(|0\rangle_\alpha + \exp\left(-2\pi i J 2^{-\alpha-1}\right) |1\rangle_\alpha\right) && \text{(3.22.12e)}
\end{aligned}$$

but in the $\exp(-2\pi i J 2^\alpha)$ the terms in the binary expansion of J with a power higher than α will just make the term rotate by 2π, doing nothing.

So, to the Least Significant Bit $|J_{n-1}\rangle$ we just apply a Hadamard. To the second LSB $|J_{n-2}\rangle$ we apply a Hadamard, and then a control-$R_z(2\pi i/2^2)$. In general

$$|J_\alpha\rangle \to \bigotimes_{k=2}^{n-\alpha} (C_{|J_{n-k+1}\rangle} - R_z)(2\pi i/2^k) \otimes H\,|J_\alpha\rangle \tag{3.22.13}$$

3.22.4 Shor's algorithm

It is a method to factor a product of large numbers.

Motivation: two-key RSA cryptography Alice wants to communicate a message P to Bob. Bob generates a public key K_{Pu} and a private key K_{Pr}, he sends the public key K_{Pu} to Alice, who encodes the message with an algorithm E which depends on the public key:

$$C = E_{K_{\mathrm{Pu}}}(P) = P^e \mod N \tag{3.22.14}$$

where N is chosen such that $N = pq$, with $p, q \in \mathbb{Z}_{\mathrm{prime}}$, $\Phi = (p-1)(q-1)$, $1 < e < \Phi$, and $\mathrm{GCD}(\Phi, e) = 1$.

The *public key* is $K_{\mathrm{Pu}} = (N, e)$; the *private key* is $K_{\mathrm{Pr}} = \Phi$ or equivalently (p, q).

She then sends C to Bob, who uses K_{Pr} to decode it with an algorithm D:

$$P = D_{K_{\text{Pr}}} C = C^d \mod N \tag{3.22.15}$$

where d is chosen such that $de = 1 \mod \Phi$.

This works because of Euler's theorem. If $\Phi(x)$ is the totient function, which returns the number of naturals $< x$ which are coprime with x, then since (unproven fact) Φ is multiplicative, $\Phi(pq) = (p-1)(q-1)$.

The theorem says that for any P, $P^\Phi \equiv 1 \mod N$. If $ed \equiv 1 \mod \Phi$ then $ed = k\Phi + 1$ for some $k \in \mathbb{N}$. So:

$$P^{ed} = P^{k\Phi+1} \equiv P \mod N \tag{3.22.16}$$

So we can decrypt our message $C = P^e$ by calculating $C^d = P^{ed}$.

In order to break the encryption we just need to factor N: if we have its factors then we can calculate Φ, after which it is easy to find a suitable d.

Factoring N is equivalent to finding the period of a function: the *order* r is the smallest number such that $x^r = 1 \mod N$: if we define a function $f(r) = x^r \mod N$, then r is also the period of that function, since the condition reads $f(r) = f(0)$.

If r is even, then $y = x^{r/2}$, so $y^2 = 1 \mod N$ therefore $(y+1)(y-1) = 0 \mod N$.

Therefore $(y+1)(y-1) = kN$ for some $k \in \mathbb{N}$, so we have found the factors.

Shor's algorithm Given $N = pq$, we have the following steps:

1. Choose $x < N$. If it divides N, we are done;
2. if they are not coprime (the check can be made quickly with Euclid's algorithm) start over;
3. find the order r of the function $f(r) = x^r \mod N$;
4. if r is even, we have the factors. If it is not, start over.

The quantum part is in step 3, which can be done using the QFT.

Hypotheses These are not actually needed but they make treating the problem much simpler, and there is not much to learn in generalizing: we assume $N = 2^n$ and $N/r = m \in \mathbb{N}$.

As always we cannot directly encode our function as a unitary transformation since it will be periodic, therefore not injective, therefore not unitary. So we encode it taking the input along, as

$$U : |x\rangle |0\rangle \longmapsto |x\rangle |f(x)\rangle \tag{3.22.17}$$

We start from $|0\rangle^{\otimes 2n}$, apply n Hadamards and get $|\psi_0\rangle$ = superposition of all possible states $\otimes |0\rangle^{\otimes n}$, and with this we prepare

$$|\psi_1\rangle = U |\psi_0\rangle = \frac{1}{\sqrt{2^n}} \sum_{x=0}^{N} |x\rangle |f(x)\rangle \tag{3.22.18}$$

Step 2 We measure the second registry, and obtain $\left|\overline{f(x_0)}\right\rangle$ for some x_0. Then the first registry must contain all the combinations which generate that state: so:

$$\left|\psi_2\right\rangle = \frac{1}{\sqrt{m}} \sum_{j=0}^{m-1} \left|x_0 + jr\right\rangle \left|\overline{f(x_0)}\right\rangle \tag{3.22.19a}$$

$$= \left[\frac{1}{\sqrt{m}} \sum_{j=0}^{m-1} \left|x_0 + jr\right\rangle\right] \otimes \left|\overline{f(x_0)}\right\rangle \tag{3.22.19b}$$

Now we can discard the last n qubits.

Step 3 We want to find r, so we can do a quantum Fourier transform. It can be slow to actually measure the full transform for generic functions but in our case the transform is applied to a function which is already periodic

$$\left|\psi_3\right\rangle = \mathrm{QFT}\Big\{\left|\psi_2\right\rangle\Big\} = \frac{1}{\sqrt{mN}} \sum_{y=0}^{N-1} \sum_{j=0}^{m-1} \exp\big(2\pi i(x_0 + jr)y/N\big) \left|y\right\rangle \tag{3.22.20}$$

Step 4 We compute the probability of obtaining a specific value $\overline{y}$ from a measure of the registry:

$$\mathbb{P}\big(\overline{y}\big) = \frac{1}{Nm} \left| \sum_{j=0}^{m-1} \exp\big(2\pi i(x_0 + jr)\overline{y}/N\big) \right| \tag{3.22.21a}$$

$$= \frac{1}{r} \left| \frac{1}{m} \sum_j \exp\big(2\pi i j\overline{y}/m\big) \right| \tag{3.22.21b}$$

where we used the fact that $N = mr$, and removed a global phase from the square.

Claim 3.22.1. *The states with nonzero probability to be found are those with $\overline{y} = km$, where $k \in 0, \dots, r$.*

Proof. If $\overline{y} = km$ then the exponential is always equal to one. Recall that $N = mr$, so we have exactly r possible values of k for which this is true, since $\overline{y} < N$.

So, for each of these we have $P(\overline{y} = km) = 1/r\left|1/m \sum_j 1\right| = 1/r$: the probability is saturated. □

So all the states we get are in the form $\overline{y} = km = kN/r$. We know N, we measured $\overline{y}$, so:

- if $k = 0$, we failed;
- if $k \neq 0$, we set $\overline{y}/N = \overline{k}/r$ and find the solution in polynomial time.

It can be shown that $\mathbb{P}(\text{success}) \sim 1$ after $O(\log(\log(r)))$ tries.

Recall $n = \log N$: the complexity of Shor's algorithm scales as $O(n^2 \log n \log\log n)$, whereas the classical algorithm scales as $\exp\Big(O(\sqrt[3]{n \log n})\Big)$.

It is important to emphasize that no classical algorithm has been found which runs in polynomial time, but it has *not* been proven that it is impossible for one to be found.

3.22.5 Phase estimation algorithm

Take a unitary transformation U such that it gives a phase to a specific autoket: $U|u\rangle = \exp(i\varphi)|u\rangle$, where $0 \leq \varphi \leq 2\pi$: we want to estimate φ.

Hypotheses We assume we are able to prepare $|u\rangle$, and that we have a blackbox $\left(C - U^{2^J}\right)$ for all $0 \leq J \leq n-1$: that is, a "control - U applied 2^J times", such that $\left(C - U^{2^J}\right)|0\rangle|u\rangle = |0\rangle|u\rangle$ and $\left(C - U^{2^J}\right)|1\rangle|u\rangle = \exp\left(i2^J\varphi\right)|1\rangle|u\rangle$.

We write φ as

$$\varphi = 2\pi\left(\frac{a}{2^n} + \delta\right) = \overline{\varphi} + \delta\varphi \tag{3.22.22}$$

with $0 \leq \delta \leq 2^{-n-1}$ and $a = a_{n-1}a_{n-2}a_{n-3}\dots a_1a_0$: we expressed it in binary, with some error.

Algorithm We introduce an ancillary registry of n qubits initialized to $|0\rangle$, while our main registry is made of m qubits, in which we encode $|u\rangle$. Their product is $\left|\psi_0\right\rangle$

We apply a H to each of the qubits in the first registry, and then the gates $\left(C - U^{2^J}\right)$ for each $0 \leq J < n$ controlling on the J-th qubit each time.

The result of this operation is $\left|\psi_1\right\rangle$. We apply a QFT to the n control bits, and the result is $\left|\psi_2\right\rangle$.

What is the result of applying $C - U^{2^J} \stackrel{\text{def}}{=} W$? It rotates u, but the phase can only be measured on the first registry:

$$\left(C - U^{2^J}\right)\left[\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes |u\rangle\right] = \frac{1}{\sqrt{2}}[W|0\rangle|u\rangle + W|1\rangle|u\rangle] \tag{3.22.23a}$$

$$= \frac{1}{\sqrt{2}}\left[|0\rangle|u\rangle + \exp\left(i2^J\varphi\right)|1\rangle|u\rangle\right] \tag{3.22.23b}$$

$$= \frac{1}{\sqrt{2}}\left[|0\rangle + \exp\left(i2^J\varphi\right)|1\rangle\right] \otimes |u\rangle \tag{3.22.23c}$$

Now we can see what is the phase by measuring the ancillary qubits, for example if the phase was just -1 we could apply a Hadamard gate and measure along the $\pm$.

So the state $\left|\psi_1\right\rangle$ is

$$\left|\psi_1\right\rangle = \frac{1}{\sqrt{2^n}}\left(\bigotimes_{J=0}^{n-1}\left(|0\rangle + \exp\left(i\varphi 2^J\right)|1\rangle\right)\right) \otimes |u\rangle \tag{3.22.24}$$

which can be written as

$$\left|\psi_1\right\rangle = \frac{1}{\sqrt{2^n}}\sum_{y=0}^{N-1}\exp(i\varphi y)|y\rangle|u\rangle \tag{3.22.25}$$

We recall

$$\mathrm{QFT}^{-1}\left\{|y\rangle\right\} = \frac{1}{\sqrt{2^n}}\sum_{x=0}^{2^n-1}\exp\left(-\frac{2\pi i x y}{2^n}\right)|x\rangle \tag{3.22.26}$$

therefore

$$\left|\psi_2\right\rangle = \mathrm{QFT}^{-1}\left|\psi_1\right\rangle = \frac{1}{2^n}\sum_{x=0}^{2^n-1}\sum_{y=0}^{2^n-1}\exp\left(2\pi i(a-x)\frac{y}{2^n}\right)\exp\left(2\pi i\delta y\right)\left|x\right\rangle\left|u\right\rangle \tag{3.22.27a}$$

so

$$\mathbb{P}(b) = \left|\left\langle b\right|\frac{1}{2^n}\sum_x\sum_y\exp\left(2\pi i(a-x)\frac{y}{2^n}\right)\exp\left(2\pi i\delta y\right)\left|x\right\rangle\right|^2 \tag{3.22.28a}$$

$$= \left|\frac{1}{2^n}\sum_y\exp\left(\frac{-2\pi iy(a-b)}{2^n}\right)\exp\left(2\pi i\delta y\right)\right|^2 \tag{3.22.28b}$$

where $\langle b| = 011101...$ from the computational basis.
Now, if the potential error $\delta = 0$, the probability of measuring "$b = a$" is just 1.
If, instead, $\delta \neq 0$, we can ask the probability of measuring $b = a$.

$$\mathbb{P}(a) = \frac{1}{2^{2n}}\left|\sum_y\exp\left(2\pi i\delta y\right)\right|^2 \tag{3.22.29a}$$

$$= \frac{1}{2^{2n}}\left|\sum_y\left(\exp(2\pi i\delta)\right)^y\right|^2 \tag{3.22.29b}$$

$$= \frac{1}{2^{2n}}\left|\frac{1-\alpha^{2^n}}{1-\alpha}\right|^2 \tag{3.22.29c}$$

$$= \frac{1}{2^{2n}}\left|\frac{1-\exp(2\pi i\delta)^{2^n}}{1-\exp(2\pi i\delta)}\right|^2 \tag{3.22.29d}$$

$$= \frac{1}{2^{2n}}\left|\frac{\sin(\pi 2^n\delta)}{\sin(\pi\delta)}\right|^2 \tag{3.22.29e}$$

So, since $\forall z \in [0,1/2] : 2z \leq \sin(\pi z) \leq \pi z$, then $\mathbb{P}a \geq 4/\pi^2 \approx 0.4$.
Actually we can achieve $\mathbb{P}(a) > 1-\varepsilon$ with $n = l + O(\log(1/\varepsilon))$.

3.22.6 Eigensolver

We want to solve the Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi \tag{3.22.30}$$

with our time evolution operator being $U(t) = \exp\left(\frac{-iHt}{\hbar}\right)$.
The eigenvalues evolve like

$$\exp\left(\frac{-iE_\alpha t}{\hbar}\right)\left|E_\alpha\right\rangle \tag{3.22.31}$$

This is a phase! we can apply the methods from before.

Spectroscopic method This is a classical method, implemented on a classical computer. There is no measurement involved, this is all done on a computer, our Hamiltonian is just a black box program.

Starting from any state $|\psi_0\rangle$, the eigenvalue equation is $H\phi_\alpha = E_\alpha \phi_\alpha$.

We can decompose our state like $\psi_0(x) = \sum_\alpha a_\alpha \phi_\alpha$. Then it evolves like

$$\psi_0(t) = \sum_\alpha a_\alpha \exp\left(\frac{-iE_\alpha t}{\hbar}\right)\phi_\alpha(x) \tag{3.22.32}$$

We can do a Fourier transform, defining $\omega_\alpha \hbar = E_\alpha$:

$$\widetilde{\psi_0}(x_0,\omega) = \int \exp(i\omega t)\sum a_\alpha \exp(-i\omega_\alpha t)\phi_\alpha(x_0)\,\mathrm{d}t \tag{3.22.33a}$$

$$= \sum_\alpha a_\alpha \int_0^T \exp\big(i(\omega-\omega_\alpha)t\big)\phi_\alpha(x)\,\mathrm{d}t \tag{3.22.33b}$$

$$\approx a_{\overline{\alpha}}\phi_{\overline{\alpha}} T + O(T^0) \tag{3.22.33c}$$

but this is peaked only at $\omega = \omega_{\overline{\alpha}}$ for large T. We can measure $a_{\overline{\alpha}}\phi_{\overline{\alpha}}T$ at different x positions, and find the eigenfunction at any point:

$$\phi_{\overline{\alpha}}(x_2) = \frac{\widetilde{\psi}(x_2,\omega_{\overline{\alpha}})}{\widetilde{\psi}(x_1,\omega_{\overline{\alpha}})}\phi_{\overline{\alpha}}(x_1) \tag{3.22.34}$$

In some cases doing this is easier than diagonalizing the Hamiltonian.

Quantizing it How to quantum-digitalize the problem? We start with a $\psi(x)$ with $x \in [-L, L]$. We can discretize the points: we divide the interval into $\Delta x = 2L/(2^n - 1)$ long steps.

Our function will then be $\psi(i) = \psi(-L + i\Delta x)$, $i \in \mathbb{N}$.

$$|\psi\rangle = \sum_{i=0}^{2^n-1} \psi(i)\,|i\rangle \tag{3.22.35}$$

We can already see that we will have exponentially less memory usage than in the classical case.

We prepare $|\psi_0\rangle = \overline{J}$. We need our infinitesimal evolution operator $U = \exp(-iH\Delta t/\hbar)$.

Our ancilla qubits are initialized to

$$\frac{1}{\sqrt{2^n}}\sum_{J=0}|J\rangle \tag{3.22.36}$$

(mapping to times $0, \Delta t, 2\Delta t, \ldots 2^{n-1}\Delta t$). With the same procedure as in 'Phase estimation algorithm' on page 79 we assume we have the control-U^{2^J} gates and apply them all. We get all the possible time evolutions:

$$\frac{1}{\sqrt{2^n}}\sum|J\rangle\, U^J\,|\psi_0\rangle = \frac{1}{\sqrt{2^n}}\sum|J\rangle\,|\psi(J\Delta t)\rangle \tag{3.22.37a}$$

$$= \frac{1}{\sqrt{2^n}}\sum|J\rangle\sum a_\alpha \exp(-i\omega_\alpha J\Delta t)\,|\phi_\alpha\rangle \tag{3.22.37b}$$

We apply QFT^{-1}, measure the first registry and get a certain eigenvalue ω_α; also, we have collapsed the second registry into the corresponding wavefunction ϕ_α, which we can then measure.

This enables us to get many eigenvalues by running this several times.

3.23 Error mitigation

Redundancy is the key to error mitigation: if the probability of error is $\varepsilon \ll 1$, if we have a duplicate the probability they both fail is proportional to $\varepsilon^2 \ll \varepsilon$.

Classical error correction Redundancy + votation.

Alice wants to send a bit of information to Bob. To prevent mistakes, she sends three. If there is a probability ε of error, and that error happens, Bob gets two equal bits and a third different bit: so he can assume that the different bit is wrong.

We have several cases, if the sent message is $0 \to 000$, shown in figure 3.2.

Number	Received message	Probability	Failure
1	000	$(1-\varepsilon)^3$	No
2	001, 010, 100	$3\varepsilon(1-\varepsilon)^2$	No
3	011, 101, 110	$3\varepsilon^2(1-\varepsilon)$	Yes
4	111	ε^3	Yes

Figure 3.2: Error correction probabilities

The probability of failure is then $O(\varepsilon^2)$.

Trying to quantize it

1. We wish to do $|\psi\rangle \to |\psi\rangle |\psi\rangle |\psi\rangle$: this is not allowed; it can be done if we can prepare the state $|\psi\rangle$ (say, it is one of the base states), but we cannot do so in general.
2. We want to do a votation: but this means we have to measure it. Maybe we can do a projection?
3. For classical bits we want to correct $|0\rangle \leftrightarrow |1\rangle$, but this is not the only possibility for quantum states.

3.23.1 3-qubit bit-flip code

We encode

$$|0\rangle \to \left|\widetilde{0}\right\rangle = |0\rangle |0\rangle |0\rangle \tag{3.23.1a}$$

$$|1\rangle \to \left|\widetilde{1}\right\rangle = |1\rangle |1\rangle |1\rangle \tag{3.23.1b}$$

and in general do

$$|\psi_1\rangle = \alpha |0\rangle + \beta |1\rangle \to \alpha \left|\widetilde{0}\right\rangle + \beta \left|\widetilde{1}\right\rangle = \alpha |0\rangle |0\rangle |0\rangle + \beta |1\rangle |1\rangle |1\rangle \tag{3.23.2}$$

This can be physically made with two CNOTs.
We did not clone the state! That would have been $(\alpha|0\rangle + \beta|1\rangle)^{\otimes 3}$.

Number	Received message	Probability	Final state
1	$\alpha\|0\rangle\|0\rangle\|0\rangle + \beta\|1\rangle\|1\rangle\|1\rangle$	$(1-\varepsilon)^3$	$\alpha\|0\rangle\|0\rangle\|0\rangle + \beta\|1\rangle\|1\rangle\|1\rangle$
2	perms. of $\alpha\|1\rangle\|0\rangle\|0\rangle + \beta\|0\rangle\|1\rangle\|1\rangle$	$3\varepsilon(1-\varepsilon)^2$	$\alpha\|0\rangle\|0\rangle\|0\rangle + \beta\|1\rangle\|1\rangle\|1\rangle$
3	perms. of $\alpha\|1\rangle\|1\rangle\|0\rangle + \beta\|0\rangle\|0\rangle\|1\rangle$	$3\varepsilon^2(1-\varepsilon)$	$\alpha\|1\rangle\|1\rangle\|1\rangle + \beta\|0\rangle\|0\rangle\|0\rangle$
4	$\alpha\|1\rangle\|1\rangle\|1\rangle + \beta\|0\rangle\|0\rangle\|0\rangle$	ε^3	$\alpha\|1\rangle\|1\rangle\|1\rangle + \beta\|0\rangle\|0\rangle\|0\rangle$

Figure 3.3: Error correction probabilities for the quantum version

We can do the correction by measuring correlations, without doing a projective measurement: $x_0 = \left\langle \sigma_z^1 \sigma_z^2 \right\rangle$, $x_1 = \left\langle \sigma_z^1 \sigma_z^3 \right\rangle$.

Why don't we collapse the state doing this?

We also get $x_0 x_1 = 00$ for the case where all the bits are flipped, but it is all right since it is $O(\varepsilon^3)$.

3.23.2 3-qubit phase-flip code

What if our error is a phase flip instead of a bit flip? Something like that could be caused by an unknown magnetic field making our state rotate, like $|0\rangle \to |0\rangle$, $|1\rangle \to -|1\rangle$. This can be corrected with a Hadamard gate, and then applying the 3 qubit-flip code.

3.23.3 9-qubit Shor code

To account for all kinds of (unitary) errors, we can use

$$|0\rangle \to \left|\widetilde{0}\right\rangle = \frac{1}{\sqrt{8}}(|000\rangle + |111\rangle)^{\otimes 3} \tag{3.23.3a}$$

$$|1\rangle \to \left|\widetilde{1}\right\rangle = \frac{1}{\sqrt{8}}(|000\rangle - |111\rangle)^{\otimes 3} \tag{3.23.3b}$$

This of course is very resource-heavy.
Experts think we should be able to achieve fault-free computation with $\varepsilon \sim 10^{-3\div 4}$.

Example We have an error like $|0\rangle \to |0\rangle$, $|1\rangle \to \exp(i\varphi)|1\rangle$.
We encode 1 of these qubits with two qubits, like $|01\rangle \equiv |0\rangle$ and $|10\rangle \equiv |1\rangle$: now these both take a phase of $\exp(i\varphi)$: we moved to a smaller subspace which is invariant under this transformation.

3.24 Time-dependent perturbation theory

We have an atom or some quantum system, and we manipulate it by sending an EM pulse against it. How will it change?

Say we have some discrete energy levels, and a continuous spectrum after some threshold energy. The photon can excite the ground state $|i\rangle$ to some excited state $|f\rangle$, or vice versa. This can happen between discrete energies, or with the continuous energies.

We need to solve the time-dep Schrödinger equation:

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\left|\psi(t)\right\rangle = \left[H_0 + \lambda W(t)\right]\left|\psi(t)\right\rangle \tag{3.24.1}$$

We work with the unperturbed eigenstates $H_0\left|\varphi_n\right\rangle = E_n\left|\varphi_n\right\rangle$, we assume $\lambda \ll 1$, and we say that the starting state at $t = 0$ is an unperturbed eigenstate.

What is the probability of getting a state f?

$$\mathbb{P}_{if}(t) = \left|\left\langle\varphi_f\middle|\psi(t)\right\rangle\right|^2 \tag{3.24.2}$$

we can get resonance. For continuous states this changes a bit but we can generalize.

We expand

$$\left|\psi(t)\right\rangle = \sum c_n(t)\left|\varphi_n\right\rangle \qquad c_n(t) = \left\langle\varphi_n\middle|\psi(t)\right\rangle \tag{3.24.3}$$

We can compute the matrix elements of the perturbation: $\left\langle\varphi_n\right| W(t)\left|\varphi_k\right\rangle = W_{nk}(t)$ and of the Hamiltonian: $\left\langle\varphi_n\right| H_0\left|\varphi_k\right\rangle = \delta_{nk}E_n$. Putting these in the Schrödinger equation, we get

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}c_n(t) = E_n c_n(t) + \sum_k \lambda W_{nk}c_k(t) \tag{3.24.4}$$

We go in interaction picture: $b_n(t) = c_n(t)\exp(+iE_nt/\hbar)$, which nullifies the unperturbed evolution. Putting this inside the equation we get

$$i\hbar\dot{b}_n(t) = \lambda\sum_k \exp(i\omega_{nk}t)W_{nk}b_k(t) \tag{3.24.5}$$

with $\omega_{nk=(E_n-E_k)/\hbar}$. We can expand the $b_n(t)$ in λ:

$$b_n(t) = \sum_i b_n^{(i)}\lambda^i(t) \tag{3.24.6}$$

We know that for some i we must have $b_n^{(r)}(t=0) = \delta_{ni}\delta_{r0}$ and so:

$$i\hbar\dot{b}_n^{(0)}(t) = 0 \tag{3.24.7}$$

$$i\hbar\dot{b}_n^{(r)}(t) = \sum_k \exp(i\omega_{nk}t)W_{nk}b_n^{r-1}(t) \tag{3.24.8}$$

Then to order λ^1:

$$i\hbar\dot{b}_n(t) = \exp(i\omega_{nk}t)W_{nk}(t) \tag{3.24.9}$$

$$b_n^{(1)}(t) = \frac{1}{i\hbar}\int_0^t \mathrm{d}\tau\exp(i\omega_{ni}\tau)W_{ni}(\tau) \tag{3.24.10}$$

So $\mathbb{P}_{if}(t) = \left|c_f(t)\right|^2 = \left|b_f(t)\right|^2$

$$\mathbb{P}_{if}(t) = \frac{\lambda^2}{\hbar^2}\left|\int_0^t \mathrm{d}\tau\exp\left(i\omega_{fi}\tau\right)W_{gi}(\tau)\right|^2 \tag{3.24.11}$$

Example Let us take a $W(t) = -W\sin(\omega t)$. Then,

$$b_n^{(1)}(t) = -\frac{W_{ni}}{2\hbar}\int_0^t \mathrm{d}\tau \left(\exp\big(i(\omega_{ni}-\omega)\tau\big) - \exp\big(-i(\omega_{ni}-\omega)\tau\big)\right) \tag{3.24.12}$$

So,

$$\mathbb{P}_{if}(t,\omega) = \frac{\left|W_{if}\right|^2}{4\hbar^2}F(t,\omega-\omega_{fi}) \tag{3.24.13}$$

where

$$F(\omega,t) = \left(\frac{\sin(\omega t/2)}{\omega/2}\right)^2 \tag{3.24.14}$$

This is a sinc squared.

3.24.1 Fermi's golden rule

Is applying what we saw to continuous spectrums. Now we have some $\langle\alpha|\alpha'\rangle = \delta(\alpha-\alpha')$. We want to see what is the probability of the final state being in a neighbourhood of α.

We define the state density by $\mathrm{d}\alpha = \rho(\beta,E)\,\mathrm{d}\beta\,\mathrm{d}E$ where the index β takes account of the degeneracy, which can be continuous.

$$\delta\mathbb{P}\Big(\alpha_f,t\Big) = \int \mathrm{d}\alpha \left|\langle\alpha|\psi(t)\rangle\right|^2 \tag{3.24.15}$$

where $\alpha \in D_f$. So, we can change variable into

$$\delta\mathbb{P}\Big(\alpha_f,t\Big) = \int \left|\langle\beta,E|\psi(t)\rangle\right|^2 \rho(E,\beta)\,\mathrm{d}E\,\mathrm{d}\beta \tag{3.24.16}$$

We can write

$$\left|\langle\beta,E|\psi(t)\rangle\right|^2 = \frac{1}{\hbar^2}\left|\langle\beta,E|\,W\,|\varphi_i\rangle\right|^2 F\left(t,\frac{E-E_i}{\hbar}\right) \tag{3.24.17}$$

where $\lim_{t\to\infty} F\Big(t,\frac{E-E_i}{\hbar}\Big) = 2\pi i\hbar\delta(E-E_i)$. Then

$$\delta\mathbb{P}(\varphi_i,\alpha_f,t) = \delta\beta_f\frac{2\pi i t}{\hbar}\left|\Big\langle\beta_f,E_f=E_i\Big|\,W\,|\varphi_i\rangle\right|^2\rho(\beta,E_f) \tag{3.24.18}$$

Then

$$W(\varphi_i,\alpha_f) = \frac{\mathrm{d}}{\mathrm{d}t}\frac{\delta\mathbb{P}}{\delta\beta} = \frac{\pi}{2\hbar}\left|\Big\langle\beta_f,E_f=E_i+\hbar\omega\Big|\,W\,|\varphi_i\rangle\right|^2\rho(\beta_f,E_f=E_i+\hbar\omega) \tag{3.24.19}$$

The more states we have in the final configuration, the greater the probability. We are assuming here that the state density is constant in the degeneracy, and we can split the degeneracy and energy contributions.

3.25 How to build a quantum computer

Di Vincenzo criteria (2000): what is needed to have a true quantum computer.

1. Scalability, well defined qubit;
2. Reset: we must be able to reset the computer surely into a state $|0\rangle$;
3. Long coherence time wrt gate duration;
4. Universal set of gates;
5. Efficient readout;

If our decoherence time is τ_d and our gate time is τ_g, we need $\tau_d/\tau_g \gtrsim 10^4$ in order to have time to do error correction.

Proposals:

- Cauidiy: QED;
- Solid-state electron spins;
- Cold atoms;
- Trapped ions;
- Superconductive circuits.

3.25.1 Trapped ions

We can trap them with electric fields: Paul trap. We cannot do the intuitive thing, because of Gausses' law. We can work around it by making them time-dependent. Think of it like this: saddle which spins, an object in the saddle point will be stable if the rotation is fast enough.

We get three harmonic oscillators, with $\omega_{x,y} \gg \omega_z$. The z direction is the 'quantum' degree of freedom: the state comes from the atom state i and the oscillator state n.

Can we put many qubits in there? Our Hamiltonian will be

$$H = \sum \frac{p_i^2}{2m} + \sum \frac{1}{2}\omega_z^2 z_i^2 + \sum_i \sum_{j<i} \frac{q^2}{4\pi\varepsilon_0 \left| r_i - r_j \right|} \tag{3.25.1}$$

They repel each other, we can diagonalize this matrix and get the modes of oscillation.

So we have $|\alpha_1 \alpha_2 \dots \alpha_N n\rangle$ where the n is the global oscillation. Our single qubit is $|\alpha_i n\rangle$. We have the states $|g,0\rangle$, $|g,1\rangle$, $|g,2\rangle$ ... and $|e,0\rangle$, $|e,1\rangle$ ...

We can use a laser to excite the ground state into a vibrational excited state... we choose the right frequency to go from $|g,k\rangle$ to $|e,k-1\rangle$ which spontaneously decays into $|g,k-1\rangle$. This is *side-band cooling*. This can prepare a state with $\mathbb{P} > 99.9\%$.

Cirac-Zoller Gate: allows us to entangle states with stuff like a CPHASE by interacting with the global vibration.

3.25.2 Superconductive qubit

Something like Bose-condensing electrons: Cooper pairs, with opposing momentums: so the entanglement is in the Fourier space, they are very delocalized in the position space. Cooper pair currents are the superconductive currents.

We use Josephson juctions inside regular circuits: two superconductors, separated by a thin insulant. Cooper pairs can tunnel through the insulant.

Charge qubit: quantum numbers inside the superconductor are n, φ, with $[n, \varphi] = i$.

$$H = E_C\Big(n - n_g\Big)^2 - E_J \cos\varphi \tag{3.25.2}$$

with $n_g - c_g V/(2e)$, and $E_C = (2e)^2/(2(C_J + C_g))$. We can write the eigenstates as $|n\rangle$, and

$$H = E_C \sum (n - n_g)\,|n\rangle\langle n| - \frac{1}{2}E_J \sum \left(|n+1\rangle\langle n| + |n\rangle\langle n+1|\right) \tag{3.25.3}$$