Handbook

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June 26, 2019

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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 $\sigma(\hat{A}) \subseteq \mathbb{R}$.

$$\sigma(A) = \left\{ a \in \mathbb{R} : \inf_{\psi \in D(A)} \Delta A_{a,\psi} = 0 \right\} \tag{1.1}$$

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:

$$\sigma(A) = \left\{ a \in \mathbb{C} : (A - a\mathbb{1})^{-1} \notin \mathcal{B}(\mathbb{R}^n) \right\} \tag{1.2}$$

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:

$$\mu\big(]a, b[\big) = \lim_{\varepsilon \to 0} g(b - \varepsilon) - g(a + \varepsilon) \tag{1.3}$$

With this we define the Lebesgue integral as usual, getting

$$\int f \,\mathrm{d}g = \int f \frac{\mathrm{d}g}{\mathrm{d}\lambda} \,\mathrm{d}\lambda \tag{1.4}$$

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 $\mathrm{d}P^A_\Sigma(\lambda)$ is the one given by applying the Riesz-Markov theorem to the linear functional $g \to \langle g(A) \rangle_\Sigma$, such that:

$$\langle A \rangle_\Sigma = \int g(\lambda) \,\mathrm{d}P^A_\Sigma(\lambda) \tag{1.5}$$

With the help of equation (1.34) we then define

$$P^A_\Sigma(\lambda) = \langle \Theta(\lambda - A) \rangle_\Sigma \tag{1.6}$$

Abstract probability measure $P^A(\lambda) = \Theta(\lambda - A)$. It allows us to abstract from equation (1.6), having

$$f(A) = \int f(\lambda) \,\mathrm{d}P^A(\lambda) \tag{1.7}$$

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

$$(\Delta A)^2_{\Sigma, a} = \langle (\lambda - a)^2 \rangle_\Sigma = \int (\lambda - a)^2 \,\mathrm{d}P^A_\Sigma(\lambda) \tag{1.8}$$

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:

$$\inf_{\psi \in D(A)} \Delta A_\psi = 0 \tag{1.9}$$

. $\langle A \rangle_\Sigma = a$ 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:

$$\|F\| = \sup_{\|\psi\|=1} F(\psi) < \infty \tag{1.10}$$

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:

$$d\Big(|\psi\rangle, |\phi\rangle\Big) = \left(1 - \frac{\left|\langle \psi | \phi \rangle\right|^2}{\|\phi\|^2 \|\psi\|^2}\right)^{1/2} \tag{1.11}$$

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

$$\sup_{\substack{\psi \in D(A) \\ \|\psi\|=1}} \left|\langle \phi | A\psi \rangle\right| < \infty \tag{1.12}$$

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 $\mathrm{d}P_\psi^A(\lambda)$ we define its pdf as:

$$W_\psi^A(\lambda) = \frac{\mathrm{d}P_\psi^A(\lambda)}{\mathrm{d}\lambda} \tag{1.13}$$

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:

$$\rho = \sum_i c_i \left| \phi_i \right\rangle \left\langle \phi_i \right| ; \qquad \sum_i c_i = 1 \tag{1.14}$$

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:

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

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

$$U(x) = \exp\left(\sum_\alpha x_\alpha e_\alpha\right) \tag{1.15}$$

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:

$$\Big(\langle\phi_1| \otimes \langle\phi_2|\Big)\Big(|\psi_1\rangle \otimes |\psi_2\rangle\Big) = \langle\phi_1|\psi_1\rangle \langle\phi_2|\psi_2\rangle \tag{1.16}$$

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.

$$\forall \phi \in \mathcal{H}_1 \otimes \mathcal{H}_2 : \phi = \sum_{m,n=0}^{\infty} c_{mn} (\phi_m^1 \otimes \phi_n^2) \tag{1.17}$$

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

$$P_\psi^A(\lambda) = \left| \langle \psi | P^A(\lambda) | \psi \rangle \right|^2 \tag{1.18}$$

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

$$U(t) = \exp\left(\frac{t\hat{H}}{i\hbar}\right) \tag{1.19}$$

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 (1.19) becomes the single eigenstate's energy. Then $|\varepsilon\rangle$ evolves like

$$\exp\left(\frac{t\varepsilon}{i\hbar}\right)|\varepsilon\rangle \tag{1.20}$$

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:

$$P^A_\Delta|\psi\rangle = \int \chi_\Delta(\lambda)\,\mathrm{d}P^A(\lambda)\,|\psi\rangle \tag{1.21}$$

where

$$\int_\Delta \mathrm{d}P^A(\lambda) = \frac{\mathbb{1}_\Delta}{\langle\psi|P^A(\Delta)|\psi\rangle} \tag{1.22}$$

(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 (1.26) 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, $\forall\psi \in C_0$:

$$f(\psi) = \int \psi(x)\,\mathrm{d}g(x) \tag{1.23}$$

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:

$$\langle\psi|A|\psi\rangle = \int \lambda\,\mathrm{d}\,\langle\psi|P(\lambda)|\psi\rangle \tag{1.24}$$

and the corresponding domain is

$$D(A) = \left\{ \psi \in \mathcal{H} : \int \lambda^2 \, \mathrm{d} \langle \psi | P(\lambda) | \psi \rangle < \infty \right\} \tag{1.25}$$

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.

$$\mathbb{1} = \sum_{\lambda_n \in \sigma_d(A)} \sum_{r=1}^{d(\lambda_n)} |\lambda_n, r\rangle\langle\lambda_n, r| + \int_{\lambda \in \sigma_c(A)} \sum_{r=1}^{d(\lambda_n)} |\lambda, r\rangle\langle\lambda, r| \tag{1.26}$$

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 $\langle U\phi | U\psi \rangle = \langle \phi | \psi \rangle$; for antilinear operators instead $\langle W\phi | W\psi \rangle = \langle \phi | \psi \rangle^*$.

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

$$A = \frac{1}{i\hbar} \frac{\mathrm{d}U}{\mathrm{d}t} \bigg|_{t=0} \in T_{\mathbb{1}}(G) \tag{1.27}$$

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:

$$U(t) = \exp\left(\frac{At}{i\hbar} \right) \tag{1.28}$$

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 (1.8), we can state the theorem:

$$\Delta A_\psi \Delta B_\psi \geq \left| \frac{\langle \psi | [A, B] | \psi \rangle}{2i} \right| \tag{1.29}$$

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:

$$\mathbb{1} = \prod_{i=1}^{n}\left(\sum_{a_i\in\sigma_d} + \int_{a_i\in\sigma_c} \mathrm{d}a_i\right)|\vec{a}\rangle\langle\vec{a}| \tag{1.30}$$

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

$$\psi(x) = U_k(x)e^{ik\cdot x} \tag{1.31}$$

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:

$$\left\langle \varepsilon_m^0 \middle| \varepsilon_n^k \right\rangle = \frac{1}{\varepsilon_n^0 - \varepsilon_m^0}\left(\left\langle \varepsilon_m^0 \middle| V \middle| \varepsilon_n^{k-1} \right\rangle - \sum_{l=1}^{k} \varepsilon_m^l \left\langle \varepsilon_m^0 \middle| \varepsilon_n^{k-l} \right\rangle\right) \tag{1.32}$$

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 $\Delta \in \mathcal{B}(\mathbb{R})$:

$$P^A_\Sigma(\Delta) = \langle \chi_\Delta \rangle_\Sigma \tag{1.33}$$

then:

$$P^A_\Sigma(]-\infty, \lambda]) = \langle \Theta(\lambda - A) \rangle_\Sigma \tag{1.34}$$

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,

$$\langle A \rangle_\psi = \sum_n \lambda_n \frac{\left| \langle \lambda_n | \psi \rangle \right|^2}{\|\psi\|^2} \tag{1.35}$$

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

$$A = \sum_n \lambda_n |\lambda_n\rangle\langle\lambda_n| \tag{1.36}$$

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

$$\langle A \rangle_\psi = \int \lambda \mathrm{d} \left\langle \psi \middle| P^A(\lambda) \psi \right\rangle = \int \lambda \mathrm{d} P^A_\psi(\lambda) \tag{1.37}$$

with

$$P^A(\lambda) = \sum_n \Theta(\lambda - \lambda_n) |\lambda_n\rangle\langle\lambda_n| \tag{1.38}$$

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

$$\frac{[A, B]}{i\hbar} \tag{1.39}$$

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:

$$D(p^2) = \left\{ \psi \in L^2 : p^2 \tilde{\psi}(p) \in L^2 \right\} \tag{1.40}$$

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

$$\|A\| = \sup_{\lambda_n \in \sigma(A)} |\lambda_n| \tag{1.41}$$

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:

$$\mathrm{d}P^A(\lambda)\Big|_{\sigma_p(A)} = \sum_{\lambda_n \in \sigma_p(A)} \delta(\lambda - \lambda_n) \sum_{r=1}^{d(\lambda_n)} |\lambda_n, r\rangle\langle\lambda_n, r| \,\mathrm{d}\lambda \tag{1.42}$$

$$\mathrm{d}P^A(\lambda)\Big|_{\sigma_c(A)} = \sum_{r=1}^{d(\lambda)} |\lambda, r\rangle\langle\lambda, r| \,\mathrm{d}\lambda \tag{1.43}$$

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 $i\hbar$:

$$\Big\{ \langle\psi|A|\psi\rangle \, , \, \langle\psi|B|\psi\rangle \Big\} = \left\langle \psi \middle| \frac{[A, B]}{i\hbar} \middle| \psi \right\rangle \tag{1.44}$$

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:

$$\partial_{tt}|\psi|^2 + \frac{\hbar}{2mi}\partial_x\big(\psi^*\partial_x\psi - \psi\partial_x\psi^*\big) = 0 \tag{1.45}$$

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

$$\mathbf{j} = \frac{\hbar}{2mi}\big(\psi^*\nabla\psi - \psi\nabla\psi^*\big) \tag{1.46}$$

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

$$\mathcal{H}_d \otimes \mathbb{C}^N \simeq \bigoplus_{j=1}^{N} \mathcal{H}_d \qquad \mathcal{H}_n \otimes \mathcal{H}_m \simeq \mathcal{H}_{m+n} \tag{1.47}$$

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:

$$e^{-A} B e^{A} = \sum_{n=0}^{\infty} \frac{1}{n!} L_A^n(B) \tag{1.48}$$

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

$$U(a) = \exp(a \cdot \nabla) = \exp\left(-\frac{a \cdot p}{i\hbar}\right) \tag{1.49}$$

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

$$\exp\left(\frac{\varphi L_3}{i\hbar}\right) x \exp\left(-\frac{\varphi L_3}{i\hbar}\right) = R(\hat{u}_3, \varphi) x \tag{1.50}$$

where $R(\hat{u}_3, \varphi)x$ is a rotation of angle φ around the z axis (by using formula (1.48)).

A generic rotation $\exp\bigl(-\varphi(L \cdot n)/i\hbar\bigr)$ 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: $J_\pm = J_1 \pm iJ_2$. Then $[J_3, J_\pm] = \hbar J_\pm$.

$$J^2 = J_\pm J_\mp \pm \hbar J_3 + J_3^2 \tag{1.51}$$

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*.

$$J_\pm |\lambda m\rangle = \hbar\sqrt{j(j+1) - m(m\pm 1)}\, |\lambda, m\pm 1\rangle \tag{1.52}$$

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

$$\Delta(L\cdot n)_\psi \Delta(L\cdot m)_\psi \geq \frac{\hbar}{2}\Big| \langle\psi|(n\wedge m)\cdot L|\psi\rangle\Big| \tag{1.53}$$

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 (1.47) 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 $\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.

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, $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ and $\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$. 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:

$$\begin{pmatrix} |\uparrow\rangle_n \\ |\downarrow\rangle_n \end{pmatrix} = \begin{pmatrix} \cos(\theta/2)e^{-i\varphi/2} & \sin(\theta/2)e^{i\varphi/2} \\ -\sin(\theta/2)e^{-i\varphi/2} & \cos(\theta/2)e^{i\varphi/2} \end{pmatrix} \begin{pmatrix} |\uparrow\rangle_3 \\ |\downarrow\rangle_3 \end{pmatrix} \tag{1.54}$$

[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:

$$\mathcal{H}_{j_1} \otimes \mathcal{H}_{j_2} = \bigoplus_{J=|j_1-j_2|}^{j_1+j_2} \mathcal{H}_J \tag{1.55}$$

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 (1.55) 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 (1.55) 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 (1.52).

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

$$\phi_\varepsilon(x) = c_1 e^{ikx} + c_2 e^{-ikx} \tag{1.56}$$

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 $L^2(\mathbb{R})$:

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int_0^\infty f_{k_0}(k)\phi_k(x) \tag{1.57}$$

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 $H = p^2/2m + m\omega^2 x^2/2 = \hbar\omega(P^2 + X^2)/2$, 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:

$$\langle X|0\rangle \propto \exp\left(-\frac{X^2}{2}\right) \tag{1.58}$$

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:

$$P^2 = X^{-2}\Big(L^2 + (X \cdot P)^2 - i\hbar(X \cdot P)\Big) \tag{1.59}$$

We then write this in polar coordinates, and find that

$$P^2 = \frac{L^2}{r^2} - \hbar^2 \frac{1}{r}\frac{\partial^2}{\partial r^2} r \tag{1.60}$$

so our radial momentum is[3]

$$P_R = -i\hbar \frac{1}{r}\frac{\partial}{\partial r} r \tag{1.61}$$

The momentum in (1.61) 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:

$$-\hbar^2 \frac{\mathrm{d}^2}{\mathrm{d}r^2}\chi_{\varepsilon l} = \left(2m(\varepsilon - U(r)) - \frac{\hbar^2 l(l+1)}{r^2}\right)\chi_{\varepsilon l} \tag{1.62}$$

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

$$h'''_{kl} + \frac{2(l+1)h''_{kl}}{r} + \left(-\frac{2(l+1)}{r^2} + k^2\right)h'_{kl} = 0 \tag{1.63}$$

And we can check that $rh_{k(l+1)}$ 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):

$$h_{kl}(r) = \sqrt{\frac{2m}{k\pi}} k(-kr)^l \left(\frac{1}{kr}\frac{\mathrm{d}}{\mathrm{d}(kr)}\right)^l \frac{\sin(kr)}{kr} \tag{1.64}$$

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

Coulomb potential We treat equation (1.62) 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:

$$\frac{\mathrm{d}^2\chi_{\varepsilon l}}{\mathrm{d}x^2} + \left(-\frac{1}{4} + \frac{\nu}{x} - \frac{l(l+1)}{x^2}\right)\chi_{\varepsilon l}(x) = 0 \tag{1.65}$$

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:

$$a_{p+1} = -a_p \frac{\nu - l - 1 - p}{(p+1)p + (p+1)(2l+2)} \sim a_p/p \tag{1.66}$$

[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 (1.66) 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:

$$L_j^k = \sum_{p=0}^{j} (-)^p \frac{(j-k)!}{(j-p)!(k+p)!j!} x^p \tag{1.67}$$

$$\chi_{nl}(x) = x^{l+1} e^{-x/2} L_{n-l-1}^{2l+1} \left(\frac{(2l+1)!(n-l-1)!}{(n+l)!} \right) \tag{1.68}$$

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: $\sigma(\theta, \varphi) = r^2 |j_d \cdot r| / |j_i|$ (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:

$$\psi(x) = \exp\left(\frac{t\varepsilon}{i\hbar}\right) \left(\exp\left(-\frac{p \cdot x}{i\hbar}\right) + \frac{f_p(\theta, \varphi)}{r} \exp\left(-\frac{pr}{i\hbar}\right) \right) \tag{1.69}$$

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:

$$\langle x|\psi\rangle = \langle x|\psi_{HOM}\rangle + \int \mathrm{d}^3y \, \langle x|\,\Omega^{-1}\,|y\rangle\langle y|\,V\,|\psi\rangle \tag{1.70}$$

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):

$$\langle x|\,\Omega^{-1}\,|y\rangle = \int \mathrm{d}^3q \, \langle x|\,\Omega^{-1}\,|q\rangle\langle q|\,|y\rangle = \int \mathrm{d}^3q \, \frac{1}{(p^2-q^2)/2m \pm i\varepsilon} \frac{e^{q\cdot(x-y)/(i\hbar)}}{\sqrt{2\pi}} \tag{1.71}$$

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.

$$\psi(x,t) = \int g_{p_0}(p) e^{\frac{\varepsilon t}{i\hbar}} \psi_{IN}(x) \mathrm{d}^3p \tag{1.72}$$

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:

$$f_P(\theta,\varphi) = -\frac{2m}{k} \int \frac{\mathrm{d}^3y}{4\pi} V(y)\psi_{IN}(y) e^{-ipr\cdot y} \tag{1.73}$$

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 $U(\sigma) |\psi\rangle = c |\psi\rangle$, 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

$$\psi(z_1, \dots, z_n) = \prod_{i<j} (z_i - z_j)^{1/3} \prod_{i=1}^{N} e^{-i|B|^2} \tag{1.74}$$

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:

$$e^{i\gamma} = \exp\left(\oint_C \langle\psi|\mathrm{d}\psi\rangle\right) \tag{1.75}$$

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 $|\psi\rangle = (|\uparrow\rangle_A |\downarrow\rangle_B - |\downarrow\rangle_A |\uparrow\rangle_B)/\sqrt{2}$.

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 $|\uparrow\rangle_A |\downarrow\rangle_B$ and $N/2$ with $|\downarrow\rangle_A |\uparrow\rangle_B$.

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:

$$B(\{u_i\}_i) = S_A \cdot u_0 \otimes (S_B \cdot u_1 - S_B \cdot u_2) + S_A \cdot u_3 \otimes (S_B \cdot u_1 + S_B \cdot u_2) \tag{1.76}$$

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 $u(\theta, \varphi) \in S^2$:

$$\langle\pm|S \cdot u|\pm\rangle = \pm\frac{\cos\theta}{2} \qquad \langle\pm|\, S \cdot u\, |\mp\rangle = \frac{1}{2}\sin\theta e^{\pm i\varphi} \tag{1.77}$$

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

$$\langle\psi|(S_A \cdot u)(S_B \cdot u')|\psi\rangle = -\frac{\cos(\theta - \theta')}{4} \tag{1.78}$$

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 $931.5\,\text{MeV}$.

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 $0.87\,\text{fm}$ for the proton, and $-0.1\,\text{fm}$ 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:

$$\rho(r) = \sum_i \left|\psi_i(r)\right|^2 \tag{2.1}$$

We can approximate it as a radial distribution

$$\rho(r) \sim \frac{\rho_0}{1 + \exp\left(\frac{r - r_0}{a}\right)} \tag{2.2}$$

where $\rho_0 \approx 0.15 \div 0.2\,\text{nucleons}/\text{fm}^3$ 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), $a \approx 0.65 \div 0.7\,\text{fm}$ is the *diffusivity*, which quantifies the length scale at which the density distribution goes to zero.

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

$$\rho_0 \approx \frac{A}{V} = \frac{A}{\frac{4}{3}\pi\left(r_0 A^{1/3}\right)^3} \approx 0.138\,\text{fm}^{-3} \tag{2.3}$$

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

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

$$M(A, Z) = Zm_p + (A - Z)m_n - B(A, Z) \tag{2.4}$$

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

$$V = \sum_{i<j} V_{ij}\left(\left|r_i - r_j\right|\right) \tag{2.5}$$

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 (2.5) 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

$$B \propto \frac{A(A-1)V_{\text{int}}}{\underbrace{V_{\text{total}}}_{\propto A}} \propto A - 1 \sim A \tag{2.6}$$

So our first term will be

$$B \sim a_V A \tag{2.7}$$

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

$$B \sim a_V A - a_S A^{2/3} \tag{2.8}$$

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

$$E(r) = \begin{cases} \frac{Zer}{4\pi\varepsilon_0 R^3} = \frac{\rho r}{4\varepsilon_0} & r \leq R \\ \frac{Ze}{4\pi\varepsilon_0 r^2} = \frac{\rho R^3}{3\varepsilon r^2} & r \geq R \end{cases} \tag{2.9}$$

The energy density of the electric field is given by $u = \varepsilon_0 E^2/2$; its integral over all of space $U = 4\pi \int_0^\infty ur^2 \, dr$, 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:

$$U = \left(1 + \frac{1}{5}\right)\frac{(Ze)^2}{8\pi\varepsilon R} \tag{2.10}$$

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:

$$B \sim a_V A - a_S A^{2/3} - a_C Z^2 A^{-1/3} \tag{2.11}$$

with

$$a_C = \frac{3}{5}\frac{e^2}{4\pi\varepsilon_0}\frac{1}{r_0} \approx 0.7\,\text{MeV} \tag{2.12}$$

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:

$$U = \frac{e^2}{4\pi\varepsilon_0} \sum_{i=1}^{Z} \sum_{j<i} \frac{1}{\left| r_i - r_j \right|} \propto \frac{Z(Z-1)}{|\overline{r}|} \propto \frac{Z(Z-1)}{A^{1/3}} \tag{2.13}$$

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

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.

$$\begin{aligned} B_A &= \frac{Nv}{A}(N+2P) + \frac{Pv}{A}(2N+P) && (2.14a)\\ &= \frac{v}{A}\left(N^2 + P^2 + 4NP\right) && (2.14b)\\ &= \frac{v}{2A}\left(3N^2 + 3P^2 + 6NP - N^2 - P^2 + 2NP\right) && (2.14c)\\ &= \frac{v}{2A}\left(3A^2 - (N-Z)^2\right) && (2.14d) \end{aligned}$$

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

$$B \sim a_V A - a_S A^{2/3} - a_C Z^2 A^{-1/3} - a_A \frac{(N-Z)^2}{A} \tag{2.15}$$

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,

$$\sum_{j=1}^{i} 2(2j+1)\Delta E = 2i^2 \Delta E = 2\frac{(N-Z)^2}{16}\Delta E \tag{2.16}$$

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

$$B_P = \frac{a_P}{A^{1/2}} \qquad a_P = \begin{cases} +\delta & \text{even-even} \\ 0 & \text{even-odd} \\ -\delta & \text{odd-odd} \end{cases} \tag{2.17}$$

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

$$B \sim a_V A - a_S A^{2/3} - a_C Z^2 A^{-1/3} - a_A \frac{(N-Z)^2}{A} \pm \frac{a_P}{A^{1/2}} \tag{2.18}$$

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*.

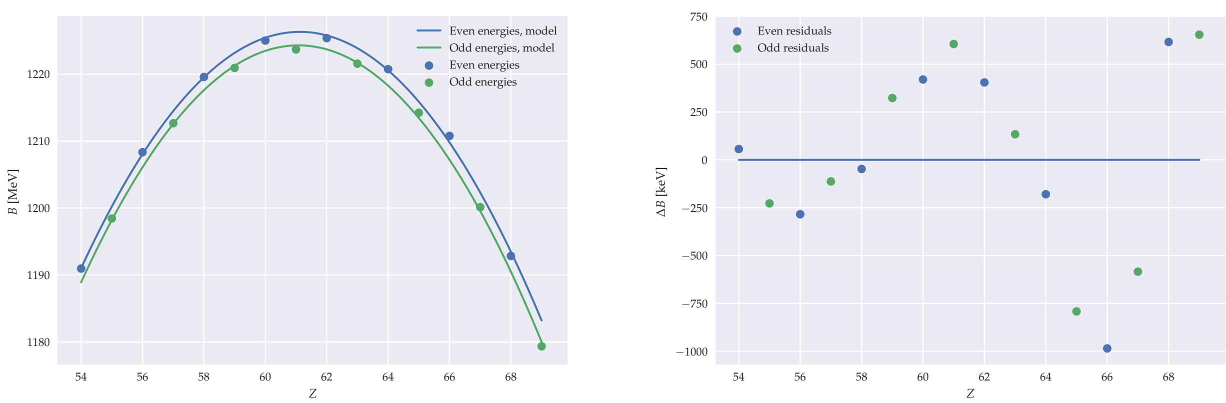
The highest binding energy per nucleon is found with ^{62}Ni ($B/A = 8.7945\,\text{MeV}$), while the lowest mass per nucleon is found with ^{56}Fe. They can be different because they have different proton/neutron ratios.

Mass parables If we work at fixed A, the (2.18) 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:

$$B = Z^2\left(-a_C A^{-1/3} - \frac{4a_A}{A}\right) + Z(4a_A) + \text{const} \tag{2.19}$$

We perform a parabolic fit for the nuclei at $A = 148$, and compute the coefficients corresponding to the fit parameters according to formula (2.19). 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 $1340\,\text{MeV}$, while the real energy is $1225\,\text{MeV}$.



(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 (2.13)) their difference in energy is given by

$$\Delta B = \frac{a_C}{A^{1/3}} \left(\frac{(A+1)(A-1)}{4} - \frac{(A-1)(A-3)}{4} \right) \tag{2.20a}$$

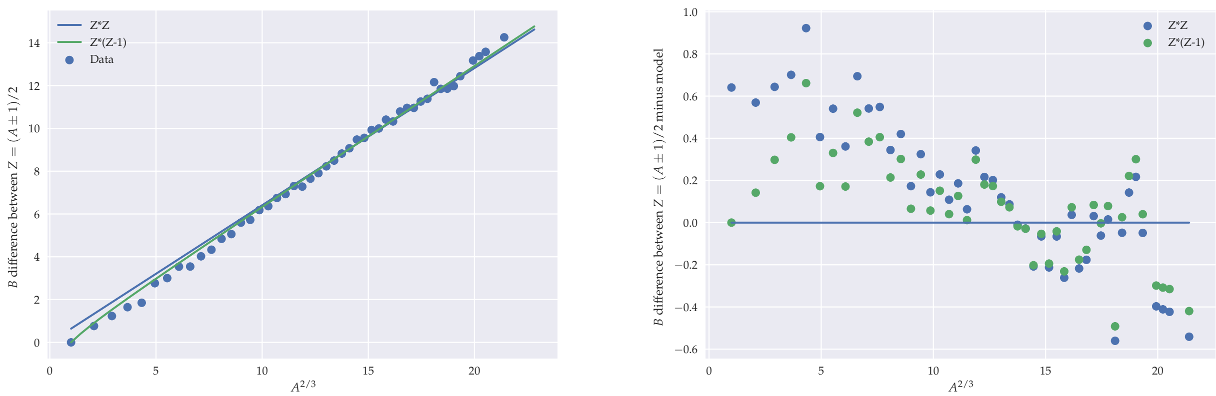
$$= \frac{a_C}{A^{1/3}} \left(\frac{4A-4}{4} \right) \tag{2.20b}$$

$$= a_C \left(A^{2/3} - A^{-1/3} \right) \tag{2.20c}$$

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

$$\Delta B = a_C x - \frac{a_C}{\sqrt{x}} \tag{2.21}$$

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

$$H = \sum_i T_i + \sum_{i<j} V_{ij}\left(\left|r_i - r_j\right|\right) \tag{2.22}$$

instead, we use

$$H_{\mathrm{sp}} = -\frac{\hbar^2 \nabla^2}{2\mu} + U(r) \tag{2.23}$$

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

$$\psi(x) = A\sin(kx) + B\cos(kx) \tag{2.24}$$

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

$$E = \frac{\hbar^2 k^2}{2m} = \frac{h^2 n_x^2}{8ma^2} \tag{2.25}$$

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

$$E = \frac{h^2}{8ma^2} \sum_i n_i^2 \tag{2.26}$$

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

$$\mathrm{d}E = \frac{h^2}{8ma^2}\,\mathrm{d}(n^2) = \frac{h^2}{4ma^2} n\,\mathrm{d}n \tag{2.27}$$

Therefore we can substitute in:

$$\rho(E)\,\mathrm{d}E = \frac{\pi}{2} \underbrace{n}_{\sqrt{8ma^2E/h^2}} \underbrace{n\,\mathrm{d}n}_{4ma^2/h^2\mathrm{d}E} = \frac{2\pi\left(2ma^2\right)^{3/2}}{h^3}\sqrt{E}\,\mathrm{d}E \tag{2.28}$$

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

$$\rho(E)\,\mathrm{d}E = \rho(p)\,\mathrm{d}p = V\frac{4\pi a^3 p^2\,\mathrm{d}p}{h^3} \tag{2.29}$$

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.

$$\mathrm{d}N = 2\rho(p)\,\mathrm{d}p = \frac{4}{3\pi}\frac{r_0^3 p^2}{\hbar^3}A\,\mathrm{d}p \tag{2.30}$$

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

$$Z = \int_0^{p_F} 2\rho(p)\,\mathrm{d}p = \int_0^{p_F} \frac{4}{3\pi}\frac{r_0^3 p^2}{\hbar^3}A\,\mathrm{d}p = \frac{4A}{9\pi}\frac{r_0^3 p_F^3}{\hbar^3} \tag{2.31}$$

Turning this around gives

$$p_F c = \frac{\hbar c}{r_0}\sqrt[3]{\frac{9\pi}{8}\frac{2Z}{A}} \tag{2.32}$$

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 (2.30). 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:

$$\langle E_k \rangle = \frac{1}{A}\int_0^A p^2/(2m)\,\mathrm{d}N = \frac{1}{A}\int_0^{p_F} \frac{p^2}{2m}\frac{4}{3\pi}\frac{r_0^3 p^2}{\hbar^3}A\,\mathrm{d}p = \frac{4}{3\pi}\frac{r_0^3}{\hbar^3}\int_0^{p_F}\frac{p^4}{2m}\,\mathrm{d}p \tag{2.33}$$

so adding their contributions we get

$$\langle E_k \rangle = \frac{4r_0^3}{3\pi\hbar^3}\left(\frac{p_{F_p}^5}{10m_p} + \frac{p_{F_n}^5}{10m_n}\right) \tag{2.34}$$

and we can substitute in the formula for the Fermi momentum (2.32), and approximate

$m \approx m_n \approx m_p$: we get

$$\langle E_k \rangle = \frac{4r_0^3}{30m\pi\hbar^3}\left(\left(\frac{\hbar}{r_0}\sqrt[3]{\frac{9\pi}{8}\frac{2Z}{A}}\right)^5 + \left(\frac{\hbar}{r_0}\sqrt[3]{\frac{9\pi}{8}\frac{2(A-Z)}{A}}\right)^5\right) \tag{2.35a}$$

$$= \frac{3^{7/3}}{80}\frac{\pi^{2/3}\hbar^2}{80Amr_0^2}\left(\left(\frac{2Z}{A}\right)^{5/3} + \left(\frac{2(A-Z)}{A}\right)^{5/3}\right) \tag{2.35b}$$

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,

$$\langle E_k \rangle = \frac{3^{7/3}}{80}\frac{\pi^{2/3}\hbar^2}{40Amr_0^2}\left(1 + \frac{5}{9}\left(\frac{2Z-A}{A}\right)^2\right) \tag{2.36}$$

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 $a = R(1+\varepsilon)$, $b = R(1+\varepsilon)^{-1/2}$.

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

The part of the SEMF that changes looks like

$$B = -a_S A^{2/3} - a_C\frac{Z^2}{A^{1/3}} + \text{const} \to -a_S A^{2/3}\left(1 + \frac{2}{5}\varepsilon^2\right) - a_C\frac{Z^2}{A^{1/3}}\left(1 - \frac{1}{5}\varepsilon^2\right) + \text{const} \tag{2.37}$$

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

$$\Delta B = A^{2/3}\left(-a_S\frac{2}{5}\varepsilon^2 + a_C\frac{Z^2}{A}\frac{1}{5}\varepsilon^2\right) = A^{2/3}\frac{\varepsilon^2}{5}\left(-2a_S + a_C\frac{Z^2}{A}\right) \tag{2.38}$$

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.

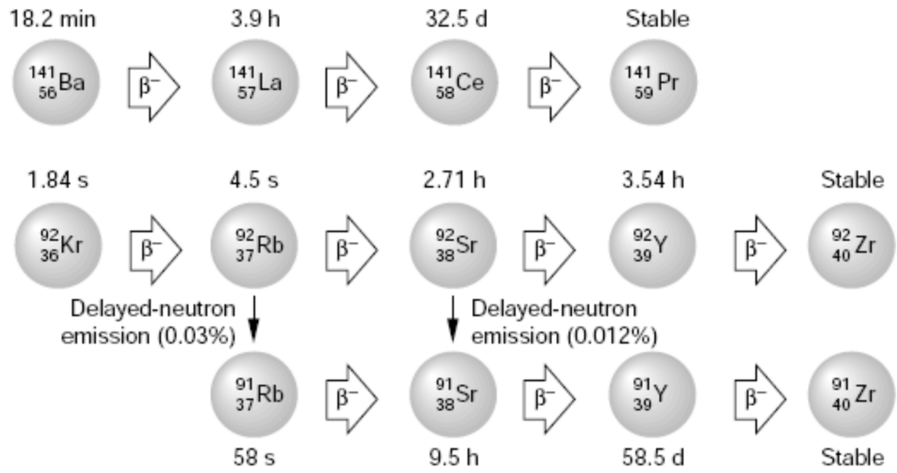


Figure 2.3: Barium decay chain

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.

$$Q = -\sum_{\text{reagents}} E_i + \sum_{\text{products}} E_i \tag{2.39}$$

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

$$V_C = \frac{e^2}{4\pi\varepsilon_0} \frac{Z_1 Z_2}{R} \tag{2.40}$$

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, $V_C \approx 500\,\text{keV}$.

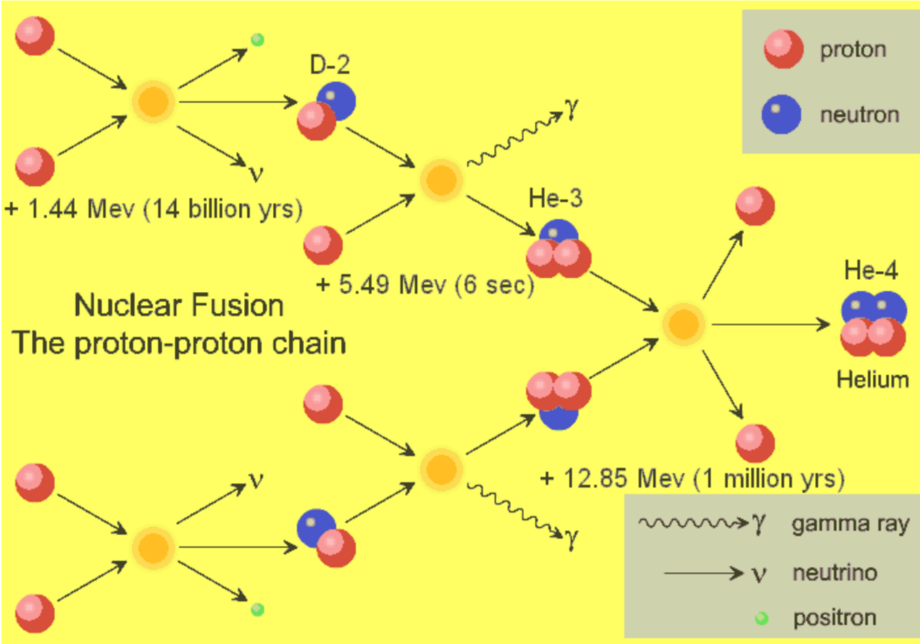


Figure 2.4: Nuclear decay chain in the Sun.

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

$$\psi(r, \Omega) = \frac{u(r)}{r} Y_{ml}(\Omega) \tag{2.41}$$

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

$$-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2 u}{\mathrm{d}r^2} + \left(V(r) + \frac{\hbar^2 l(l+1)}{2\mu r^2} \right) u(r) = Eu(r) \tag{2.42}$$

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

$$P^2 = \frac{L^2}{r^2} - \hbar^2 \frac{1}{r}\frac{\partial^2}{\partial r^2} r \tag{2.43}$$

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 $j^\pi = +1$

$$(+)(+)(-)^L = (+) \qquad 1 = \vec{L} + \vec{S} \tag{2.44}$$

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

$$\vec{\mu} = \frac{e\hbar}{2m}\vec{L} + \sum g_S \mu_N \vec{S} = (g_L^p + g_L^n)\mu_N \vec{L} + (g_S^p \vec{S}_p + g_S^n \vec{S}_n)\mu_N \tag{2.45}$$

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 $Q \approx 3\,\text{meb}$, 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

$$D(N) = \sum_{\substack{L \leq N \\ N+L \equiv 0 \mod 2}} 2(2L+1) \tag{2.46}$$

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:

$$V_{\text{WS}} = \frac{-V_0}{1+\exp\left(\frac{r-r_0}{a}\right)} \tag{2.47}$$

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.

$$E_{\text{spin-orbital}} = k\frac{\mathrm{d}V_{\text{WS}}}{\mathrm{d}r} L \cdot S \tag{2.48}$$

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).

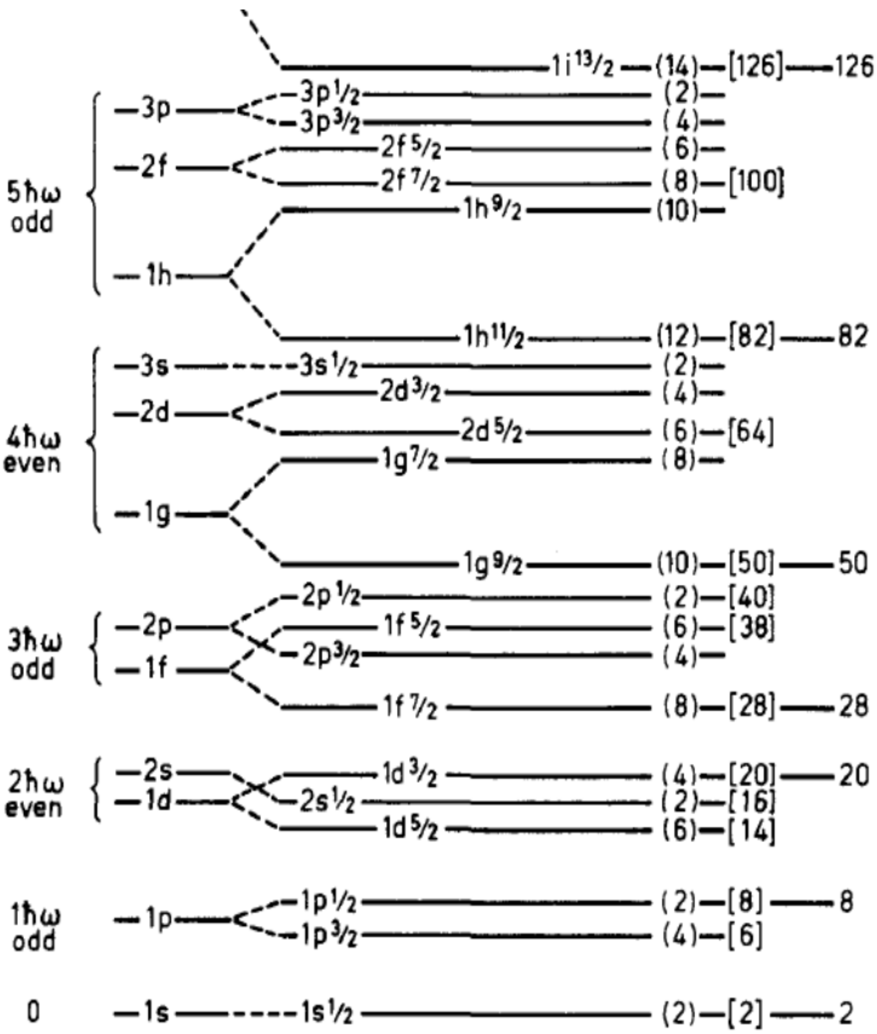


Figure 2.5: One-particle orbits

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

$$R(\theta, \varphi) = R_0 \left(1 + \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \alpha_{lm} Y_{lm}(\theta, \varphi) \right) \tag{2.49}$$

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 $a_{20} = \beta \cos(\gamma)$,

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

$$\mathcal{D}^{j}_{mm'}(\alpha, \beta, \gamma) = \left\langle jm' \middle| \exp(-i\alpha J_z) \exp\left(-i\beta J_y\right) \exp(-i\gamma J_z) \middle| jm \right\rangle \tag{2.50}$$

$a_{2(\pm 2} = \beta \sin(\gamma)/\sqrt{2}$. 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

$$R_k = R_0 \left(1 + \frac{5}{4\pi}\beta\cos\left(\gamma + \frac{2}{3}\pi k\right)\right) \tag{2.51}$$

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

$$H = \frac{\pi_{2\mu}\pi^\dagger_{2\mu}}{2B} + \frac{C}{2}\alpha_{2\mu}\alpha^\dagger_{2\mu} \tag{2.52}$$

and we have expressions for B, C.

The solutions for the Hamiltonian (2.52) 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

$${}^A_Z X \to {}^{A-4}_{Z-2} Y + \alpha \tag{2.53}$$

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 $Q = p^2_\alpha/2m_\alpha + p^2_Y/2m_Y$, 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* (2.54). It is very closely followed if we fix an even Z and vary N keeping it even as well.

$$\log(t_{1/2}) \propto ZQ^{-1/2} \tag{2.54}$$

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 $\mathbb{P}_{\text{formation}} = \left|\langle\psi(A,Z)|\left(|\psi(A-4, Z-2)\rangle \otimes |\psi(4,2)\rangle\right)\right|^2$.

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

$$V(r) = \frac{e^2}{4\pi\varepsilon_0}\frac{Z_Y Z_\alpha}{r}[r \geq R] - V_0[0 \leq r < R] \tag{2.55}$$

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,

$$T = \exp\left(-2\int_R^b \sqrt{\frac{2m(V(r)-Q)}{\hbar^2}}\,\mathrm{d}r\right) \tag{2.56}$$

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

$$G = 2\frac{Ze^2}{\hbar c}\sqrt{\frac{2m_\alpha c^2}{Q}}\left(\arccos\left(\sqrt{\frac{Q}{B}}\right) - \sqrt{\left(\frac{Q}{B}\right)\left(1-\frac{Q}{B}\right)}\right) \tag{2.57}$$

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: $\mathbb{P}_{\text{formation}} \sim 1$, $f \sim 10^{21}$ 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

$$\lambda = \frac{2\pi}{\hbar} |M|^2 \frac{\mathrm{d}n}{\mathrm{d}E} \tag{2.58}$$

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 (2.29). Then

$$\mathrm{d}n = \left(\frac{4\pi V}{h} \right)^3 p_e^2 \,\mathrm{d}p_e \, p_\nu^2 \,\mathrm{d}p_\nu \tag{2.59}$$

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

$$\mathrm{d}n = \left(\frac{4\pi V}{h} \right)^3 \frac{\mathrm{d}E_0}{c} \frac{(E_0 - E_e)^2}{c^2} p_e^2 \,\mathrm{d}p_e \tag{2.60}$$

Calculation of λ We can plug this (with the $\mathrm{d}E_0$ brought to the left hand side) into equation (2.58), 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 $p_e + \mathrm{d}p_e$.

$$\mathrm{d}\lambda = \frac{2\pi}{\hbar} |M|^2 \left(\frac{4\pi V}{h} \right)^3 F(Z_Y, E_e) \frac{(E_0 - E_e)^2}{c^3} p_e^2 \,\mathrm{d}p_e = |M|^2 \frac{(4\pi V)^3}{c^3 h^4} F(Z_Y, E_e) (E_0 - E_e)^2 p_e^2 \,\mathrm{d}p_e \tag{2.61}$$

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.

$$\lambda = |M|^2 \frac{(4\pi V)^3}{c^3 h^4} F(Z_Y, E_e) \int (E_0 - E_e)^2 p_e^2 \left[0 \leq (p_e c)^2 \leq E_0^2 - m_e^2 c^4 \right] \mathrm{d}p_e \tag{2.62}$$

Fermi-Kurie plot Flipping equation (2.61) around, we find that

$$K(E_e) = \sqrt{\frac{\mathrm{d}\lambda}{\mathrm{d}p_e} F^{-1} p_e^{-2}} \propto E_0 - E_e \tag{2.63}$$

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 $p_\nu^2 = (E_0 - E_e) \sqrt{(E_0 - E_e)^2 - m_\nu^2 c^4} / c^2$). This allows us to measure the neutrino mass.

From equation (2.62) we can calculate $ft \stackrel{\text{def}}{=} F(Z_Y, E_e) \log(2) / \lambda$. 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:

$$M = \int \psi_\nu^* \psi_e^* \psi_{\text{nuc - f}}^* \psi_{\text{nuc - i}}\, \mathrm{d}r \tag{2.64}$$

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

$$\vec{I}_i = \vec{I}_f + \vec{L} + \vec{S} \tag{2.65}$$

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:

$$E_\gamma = M\left(-1 \pm \sqrt{1 + \frac{\Delta E}{M}}\right) \approx \Delta E - \frac{\Delta E^2}{M} \approx \Delta E \tag{2.66}$$

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

$$EL \iff \Delta\pi = (-)^L \qquad ML \iff \Delta\pi = (-)^{L+1} \tag{2.67}$$

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 $\sigma = E, M$:

$$P(\sigma L) = \frac{2c}{\varepsilon_0} \frac{(L+1)}{L((2L+1)!!)^2} \left(\frac{\omega}{c}\right)^{2L+2} \mathcal{M}(\sigma L)^2 \tag{2.68}$$

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

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

$$T(\sigma L) = \frac{8\pi\alpha c(L+1)}{e^2 L(2L+1)!!^2} \left(\frac{\omega}{c}\right)^{2L+1} \left|\mathcal{M}(\sigma L)\right|^2 \tag{2.69}$$

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):

$$\left|\mathcal{M}(EL)\right|^2/e^2 = \frac{1}{4\pi}\left(\frac{3}{3+L}\right)^2 (r_0 A^{1/3})^{2L} \tag{2.70a}$$

$$\left|\mathcal{M}(ML)\right|^2 \propto \left(\frac{3}{3+L}\right)^2 (r_0 A^{1/3})^{2L-2} \tag{2.70b}$$

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

$$T(EL) \approx \frac{2\alpha(L+1)}{L(2L+1)!!^2} \left(\frac{\omega}{c}\right)^{2L+1} \left(\frac{3}{3+L}\right)^2 R^{2L} \tag{2.71}$$

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 : $\sigma \sim Z^{4\div 5}/E_\gamma^3$, for $E_\gamma < 400\,\text{keV}$.

Compton : continuous spectrum,

$$E'_\gamma = \frac{E_\gamma}{1 + (E_\gamma/m_e c^2)(1-\cos(\theta))} \qquad \text{or} \qquad \frac{1}{E'_\gamma} - \frac{1}{E_\gamma} = \frac{m}{1-\cos(\theta)} \tag{2.72}$$

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

$$E_e = \frac{4 m_e E_\alpha}{M_\alpha} \tag{2.73}$$

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,

$$\frac{ze}{\varepsilon_0} = \int E_\perp \,\mathrm{d}x\, b\,\mathrm{d}\theta = \int eE 2\pi b\,\mathrm{d}x \tag{2.74}$$

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

$$\Delta p_\perp = \int eE\,\mathrm{d}t = \int eE \frac{2\pi b}{2\pi b}\frac{\mathrm{d}x}{v} = \frac{ze}{\varepsilon_0}\frac{e}{2\pi b v} \tag{2.75}$$

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 $n = Z N_A \rho/A$ 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:

$$-\Delta E = \int \left(\frac{ze}{\varepsilon_0} \frac{e}{2\pi b v} \right)^2 \frac{1}{2m_e} \frac{Z N_A \rho}{A} 2\pi b \, \mathrm{d}b \, \mathrm{d}x \tag{2.76a}$$

$$-\frac{\mathrm{d}E}{\mathrm{d}x} = \left(\frac{ze^2}{4\pi\varepsilon_0} \right)^2 \frac{4\pi Z N_A \rho}{m_e v^2 A} \int \frac{\mathrm{d}b}{b} \tag{2.76b}$$

$$-\frac{\mathrm{d}E}{\mathrm{d}x} = \left(\frac{ze^2}{4\pi\varepsilon_0} \right)^2 \frac{4\pi Z N_A \rho}{m_e v^2 A} \log \left(\frac{m_e v^2}{h \langle \nu_e \rangle} \right) \tag{2.76c}$$

where we used $b_{\text{max}} = 2v / \langle \nu_e \rangle$, since if the time it takes the electron to oscillate $(1/ \langle \nu \rangle)$ 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 $b_{\text{min}} = h/p_e = h/(m_e v)$ since then the particle will pass *through* the electron, and quantum stuff will happen. We introduce $I = h \langle \nu \rangle$ as the ionization potential of the material, and some terms coming from relativistic considerations

$$S = -\frac{\mathrm{d}E}{\mathrm{d}x} = \left(\frac{ze^2}{4\pi\varepsilon_0} \right)^2 \frac{4\pi Z N_A \rho}{m_e v^2 A} \left(\log \left(\frac{2 m_e v^2}{I(1-\beta^2)} \right) - \beta^2 \right) \tag{2.77}$$

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

$$R = \int \frac{\mathrm{d}x}{\mathrm{d}E} \, \mathrm{d}E = \int_0^{E_0} \frac{\mathrm{d}E}{-S} \tag{2.78}$$

plugging in a rough version of formula (2.77) (we get this by dividing and multiplying by M, the mass of the particle): $S \approx azE^{-1} = 2azM/E$. Then

$$R \approx \frac{1}{2a} \frac{E_0^2}{z^2 M} \tag{2.79}$$

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 positive: the ket can always be written as

$$|\psi\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + \sin\left(\frac{\theta}{2}\right)e^{i\varphi}|1\rangle \tag{3.1}$$

with $\varphi \in [0, 2\pi]$ and $\theta \in [0, \pi]$: these can be interpreted as angles on a sphere.

We can use an n-qubit system:

$$|\psi\rangle = \sum_{i=0}^{2^n-1} a_i |i\rangle \tag{3.2}$$

where $|i\rangle$ is a base state of the tensor product space of the n Hilbert spaces: $|i\rangle = |\alpha_0\rangle_0 \otimes |\alpha_1\rangle_1 \otimes \dots |\alpha_{n-1}\rangle_{n-1}$; the α_j are the components of the representation of i in binary: $\alpha_0\alpha_1 \dots \alpha_{n-1}$ (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 $|\psi\rangle = |\psi_A\rangle_A \otimes |\psi_B\rangle_B$.

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

Lemma: they can be decomposed into smaller *quantum gates*, which are $2n \times 2n$ complex unitary matrices.

3.2 Quantum gates

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 $|-\rangle = H|1\rangle \propto |0\rangle - |1\rangle$.

$$H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \tag{3.3}$$

Phase It is a *one-qubit gate* which gives a phase to a state: applying it to a generic qubit, written as (3.1), we get $R_z(\delta)\,|\psi\rangle = \cos(\theta/2)\,|0\rangle + \exp\big(i(\varphi+\delta)\big)\sin(\theta/2)\,|1\rangle$.

$$R_z(\delta) = \exp(i\delta\sigma_z) = \begin{pmatrix} 1 & 0 \\ 0 & \exp(i\delta) \end{pmatrix} \tag{3.4}$$

State generation We can get any state $|\psi\rangle$ written as (3.1) with Hadamard and phase-shift:

$$\begin{aligned}
|\psi\rangle &= R_z(\pi/2+\varphi)HR_z(\theta)H\,|0\rangle & \text{(3.5a)}\\
&= \frac{1}{2}\begin{pmatrix} 1+e^{i\theta} \\ i\left(e^{i\varphi} - e^{i(\theta+\varphi)}\right) \end{pmatrix} & \text{(3.5b)}\\
&= \frac{1}{2}\begin{pmatrix} e^{i\theta/2} + e^{-i\theta/2} \\ i^{-1}\left(e^{i\theta/2} - e^{-i\theta/2}\right)e^{i\varphi} \end{pmatrix} & \text{(3.5c)}\\
&= \begin{pmatrix} \cos(\theta/2) \\ \sin(\theta/2)e^{i\varphi} \end{pmatrix} & \text{(3.5d)}
\end{aligned}$$

where in the step (3.5c) we used the fact that a quantum state is only defined up to a phase, and multiplied by $\exp(-i\theta/2)$.

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

$$\text{CNOT} = \begin{pmatrix} 1 & 0 & & \\ 0 & 1 & & \\ & & 0 & 1 \\ & & 1 & 0 \end{pmatrix} \tag{3.6}$$

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*:

$$\text{CPHASE}(\delta) = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & R_z(\delta) \end{pmatrix} \tag{3.7}$$

where we used the phase gate (3.4).

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:

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

$$U_f\,|x\rangle\,|y\rangle = |x\rangle\,|y \oplus f(x)\rangle \tag{3.8}$$

where $\oplus$ is bitwise XOR.

3.2.1 Parallelism

3.2.2 No cloning