

Chapter 1

Quantum Chaos

1.1 Fundamental notions

In this section will briefly present the basic principles of quantum mechanics and introduce the concepts which are required for the characterisation of energy spectra. We begin with the concept of the physical state. A *physical state* contains all the information that can be learned about the system. We associate to our physical system a *Hilbert space*, denoted with \mathbb{H} , which will contain all the possible states of the system. A vector in the Hilbert space will describe the state of the system (more rigorously only the direction of the vector will describe the state since by convention any two vectors that differ only by a constant describe the same physical state). In the Dirac formalism [1] the vectors in the Hilbert space corresponding to physical states are represented by *ket vectors*, denoted with $|\Psi\rangle$. The elements of the dual of the Hilbert space are called *bra vectors* and are denoted with $\langle\Psi|$. Due to the isomorphism between the Hilbert space and its dual, the bra vectors equally describe the physical state and the correspondence between the ket vectors and the bra vectors is given by dual conjugation.

The observables postulate

In quantum mechanics the properties of the physical system, called *observables* are described by linear hermitian operators. As a result of a measurement, the obtained values of the observable are among the eigenvalues of the associated hermitian operator.

The measurement postulate

Let us consider a physical system in a state described by the state vector $|\Psi\rangle \in \mathbb{H}$ and an observable described by the linear hermitian operator A . If a measurement of the observable is performed, then following the measurement the system will jump in an uncontrollable manner in one of the eigenstates of the operator associated with the measured observable and the result of the measurement will be given by the corresponding eigenvalue. The probability of obtaining a given eigenvalue is

given by the square of the absolute value of the scalar product between the final state associated with the given eigenvalue and the initial state.

Fundamental commutation relations

In analogy with classical mechanics, a quantum version of the Poisson brackets can be defined, postulating that they have the same properties as the classical Poisson brackets, namely anti-symmetry, linearity, the product rule and the Jacobi identity. These properties uniquely define the form of the quantum Poisson brackets the commutator of two observables, $[A, B] = AB - BA$, as being proportional to the quantum Poisson brackets

$$[A, B] = i\hbar\{A, B\}_{QM}.$$

Thus we obtain the fundamental commutation relations in quantum mechanics

$$\begin{aligned}[Q_i, Q_j] &= 0 \\ [P_i, P_j] &= 0 \\ [Q_i, P_j] &= i\hbar\delta_{i,j}.\end{aligned}$$

Time evolution postulate

In quantum mechanics time is just a parameter and not an observable. The time evolution can be postulated in different ways. If we consider the states as time dependent entities and observables as time independent ones, we can view the time evolution as a temporal displacement, similar to a spatial displacement. Then we can use the time evolution operator identity

$$i\hbar\frac{\partial}{\partial t}U(t, t_0) = HU(t, t_0)$$

to derive the Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}|\Psi\rangle = H|\Psi\rangle.$$

If we consider the states as time independent and the observables as time dependent, then the time evolution of the observables will be given by

$$i\hbar\frac{d}{dt}A(t) = [A(t), H].$$

We can observe the link between this equation and Hamilton's equations is given by the correspondence between the commutator in quantum mechanics and the Poisson bracket in classical mechanics, as mentioned in the previous chapter.

The first approach is called the Schrödinger picture of quantum mechanics, while the second is called the Heisenberg picture. There is also another formulation, namely the interaction picture also named the Dirac picture. In the following we will only consider the Schrödinger picture.

In the particular case when the Hamiltonian is time-independent, Schrödinger's equation reduces to

$$H|\Psi\rangle = E|\Psi\rangle,$$

also called the time-independent Schrödinger equation and the time evolution of the state is given by

$$|E(t)\rangle = e^{-\frac{i}{\hbar}(t-t_0)H} |E(t_0)\rangle = e^{-\frac{i}{\hbar}(t-t_0)E} |E\rangle.$$

Thus if the system is initially in an energy eigenstate, it will remain in the same state, having at most a phase modulation. Such states are called *stationary states*.

1.2 From symmetry to degeneracy

Let us consider the above mentioned time-independent case. If we suppose that the energy spectrum is discrete,

$$H|\Psi_i\rangle = E_i|\Psi_i\rangle.$$

If for an eigenvalue E_i repeats itself for different eigenstates $|\Psi_i\rangle$ we have what is called a *degeneracy*. In order to emphasise this, we can use a second index for the eigenvectors, $j = 1, \dots, m$, where m is the number of times the eigenvalue repeats.

Thus for the i -th eigenvalue,

$$H|\Psi_{i,j}\rangle = E_i|\Psi_{i,j}\rangle.$$

If the Hamiltonian is invariant to a set of unitary transformations, $T^\dagger H T = H$, then this set forms a group since the transformation given by TT' , with T' an arbitrary transformation from the set, will also leave the Hamiltonian invariant. Since symmetry operations form a group, the unitary operators which correspond to the symmetries of the Hamiltonian will form a group to which the Hamiltonian is invariant. Thus,

$$TH = TT^\dagger HT = TT^{-1}HT = HT,$$

or $[T, H] = 0$. We can once again observe how classical mechanics and quantum mechanics are linked through the Poisson bracket-commutator structure. In classical mechanics Noether's theorem asserts that to any symmetry of the action will correspond a constant of the motion. This will have a vanishing Poisson bracket with the Hamiltonian. For example, the invariance to rotations around a given axis will lead to angular momentum conservation.

Since the operators commute, they share a common set of eigenvectors

$$H(T|\Psi_i\rangle) = HT|\Psi_i\rangle = TH|\Psi_i\rangle = TE_i|\Psi_i\rangle = E_i(T|\Psi_i\rangle).$$

Thus if the Hamiltonian is invariant to the set of unitary transformations $\{T_j\}$, with $j = 1, \dots, m$

$$T_j H |\Psi_i\rangle = T_j E_i |\Psi_i\rangle = E_i (T_j |\Psi_i\rangle) = E_i |\Psi_{i,j}\rangle$$

and we will not change the value of the eigenvalue E_i by applying T_j , we only transform the eigenstates $|\Psi_i\rangle$ to a linear combination $|\Psi_{i,j}\rangle$.

1.3 Level repulsion

As is the case with classical mechanics there are few situations in which the analytic solution is known. In order to find approximate solutions we can use perturbation theory if we can assume that the Hamiltonian can be viewed as to have a part for which the solutions are known and another part that can be considered a small perturbation. The following concepts are mainly following the notations from [2] and the lecture notes [3, 4].

In the framework of time-independent perturbation theory, we want to obtain an approximate solution to the problem

$$H |\Psi^{[j]}\rangle = E_j |\Psi^{[j]}\rangle \quad (1.1)$$

and we consider that the Hamiltonian can be written as $H = H_0 + \lambda V$, where the solution to the unperturbed problem

$$H_0 |\Psi_{n\alpha}^0\rangle = E_n^0 |\Psi_{n\alpha}^0\rangle$$

is known and α gives the degeneracy of the n -th level.

Since the unperturbed eigenvectors form a basis in the Hilbert space, we can expand the perturbed eigenvectors in that basis.

$$|\Psi^{[j]}\rangle = \sum_{m,\beta} c_{m,\beta}^{[j]} |\Psi_{m,\beta}^0\rangle.$$

Inserting into eq. (1.1) we obtain

$$(H_0 + \lambda V) \sum_{m,\beta} c_{m,\beta}^{[j]} |\Psi_{m,\beta}^0\rangle = \sum_{m,\beta} E_j c_{m,\beta}^{[j]} |\Psi_{m,\beta}^0\rangle.$$

Using the solution to the unperturbed problem the above equation becomes

$$\sum_{m,\beta} (E_m^0 + \lambda V) c_{m,\beta}^{[j]} |\Psi_{m,\beta}^0\rangle = \sum_{m,\beta} E_j c_{m,\beta}^{[j]} |\Psi_{m,\beta}^0\rangle.$$

To simplify the discussion we will now consider what happens with two unperturbed states $|\Psi_1^0\rangle$ with the energy E_1^0 and $|\Psi_2^0\rangle$ with the energy E_2^0 when $\lambda = 1$.

$$\sum_{m,\beta} (E_m^0 + V) c_m^{[j]} |\Psi_m^0\rangle = \sum_{m=1,2} E_j c_m^{[j]} |\Psi_m^0\rangle.$$

By taking the scalar product with the state $\langle \Psi_k^0 |$ and using the orthogonality relation $\langle \Psi_k^0 | \Psi_m^0 \rangle = \delta_{k,m}$ we obtain

$$E_k^0 c_k^{[j]} + \sum_{m=1,2} \langle \Psi_k^0 | V | \Psi_m^0 \rangle c_m^{[j]} = E_j c_k^{[j]},$$

or

$$c_k^{[j]} (E_k^0 - E_j + V_{k,k}) + \sum_{m \neq k} V_{k,m} c_m^{[j]} = 0,$$

where $\langle \Psi_k^0 | V | \Psi_m^0 \rangle \equiv V_{k,m}$.

The above equation becomes

$$\begin{aligned} (E_1^0 - E_j + V_{1,1}) c_1^{[j]} + V_{1,2} c_2^{[j]} &= 0, \text{ for } k = 1 \\ V_{2,1} c_1^{[j]} + (E_2^0 - E_j + V_{2,2}) c_2^{[j]} &= 0, \text{ for } k = 2. \end{aligned}$$

We use the following notations:

$$H_{1,1} \equiv E_1^0 + V_{1,1}, H_{2,2} \equiv E_2^0 + V_{2,2}, H_{1,2} \equiv V_{1,2}, H_{2,1} \equiv V_{2,1}, \delta \equiv H_{1,1} - H_{2,2}, \tan \beta \equiv \frac{2|H_{1,2}|}{\delta}.$$

The above system of equations has non-trivial solutions if the determinant vanishes.

$$(H_{1,1} - E_j)(H_{2,2} - E_j) - H_{1,2}H_{2,1} = 0$$

or

$$E_j^2 - (H_{1,1} + H_{2,2})E_j + H_{1,1}H_{2,2} - H_{1,2}H_{2,1} = 0.$$

This equation has the solutions

$$E_j = \frac{(H_{1,1} + H_{2,2}) \pm \sqrt{(H_{1,1} + H_{2,2})^2 - 4(H_{1,1}H_{2,2} - H_{1,2}H_{2,1})}}{2} \quad (1.2)$$

$$= \frac{H_{1,1} + H_{2,2}}{2} \pm \frac{1}{2} \sqrt{\delta^2 + 4|H_{1,2}|^2}. \quad (1.3)$$

Since $(H_{1,1} - E_j) c_1^{[j]} + H_{1,2} c_2^{[j]} = 0$,

$$\frac{c_1^{[j]}}{c_2^{[j]}} = \frac{H_{1,2}}{E_j - H_{1,1}}.$$

If we rewrite eq. (1.3) as

$$E_j = \frac{1}{2} \left[H_{1,1} + H_{2,2} \mp (H_{2,2} - H_{1,1}) \sqrt{1 + \frac{4|H_{1,2}|^2}{\delta^2}} \right]$$

we obtain

$$\frac{c_1^{[j]}}{c_2^{[j]}} = \frac{2H_{1,2}}{H_{2,2} - H_{1,1}} \left[1 \mp \sqrt{1 + \frac{4|H_{1,2}|^2}{\delta^2}} \right]^{-1} = -\tan \beta \left(1 \mp \sqrt{1 + \tan^2 \beta} \right).$$

This ratio can be also expressed as

$$\begin{aligned} \frac{c_1^{[j]}}{c_2^{[j]}} &= \frac{-\tan \beta}{1 \mp \frac{1}{\cos \beta}} = \frac{-\sin \beta}{\cos \beta \mp 1} \\ &= \frac{-2 \sin \frac{\beta}{2} \cos \frac{\beta}{2}}{\cos^2 \frac{\beta}{2} - \sin^2 \frac{\beta}{2} \mp (\cos^2 \frac{\beta}{2} + \sin^2 \frac{\beta}{2})} = \begin{cases} \cot \frac{\beta}{2} \\ -\tan \frac{\beta}{2} \end{cases}. \end{aligned}$$

Thus,

$$\begin{aligned} |\Psi^{[1]}\rangle &= \cos \frac{\beta}{2} |\Psi_1^0\rangle + \sin \frac{\beta}{2} |\Psi_2^0\rangle \\ |\Psi^{[2]}\rangle &= -\sin \frac{\beta}{2} |\Psi_1^0\rangle + \cos \frac{\beta}{2} |\Psi_2^0\rangle. \end{aligned}$$

If the matrix elements of the interaction which mix distinct states are relatively small, that is $|H_{1,2}| \ll \delta$, $\beta \simeq 0$

$$E_{1,2} = \frac{H_{1,1} + H_{2,2}}{2} \pm \frac{\delta}{2} \sqrt{1 + \frac{4|H_{1,2}|^2}{\delta^2}}$$

Thus

$$E_1 \simeq H_{1,1} + \frac{|H_{1,2}|^2}{\delta}$$

and

$$E_2 \simeq H_{2,2} - \frac{|H_{1,2}|^2}{\delta}.$$

and the perturbed energy levels are close to the unperturbed ones. The states will also be approximatively the unperturbed ones

$$\begin{aligned} |\Psi^{[1]}\rangle &\simeq |\Psi_1^0\rangle \\ |\Psi^{[2]}\rangle &\simeq |\Psi_2^0\rangle. \end{aligned}$$

If on the other hand, the matrix elements levels which mix distinct states are relatively strong, that is $|H_{1,2}| \gg \delta$, $\beta \simeq \frac{\pi}{2}$

$$E_{1,2} = \frac{H_{1,1} + H_{2,2}}{2} \pm \sqrt{\frac{\delta^2}{4} + |H_{1,2}|^2} \simeq \frac{H_{1,1} + H_{2,2}}{2} \pm \left(|H_{1,2}| + \frac{\delta^2}{8|H_{1,2}|} \right)$$

and

$$\begin{aligned} |\Psi^{[1]}\rangle &\simeq \frac{\sqrt{2}}{2} |\Psi_1^0\rangle + \frac{\sqrt{2}}{2} |\Psi_2^0\rangle \\ |\Psi^{[2]}\rangle &\simeq -\frac{\sqrt{2}}{2} |\Psi_1^0\rangle + \frac{\sqrt{2}}{2} |\Psi_2^0\rangle. \end{aligned}$$

In this case we observe that if $\delta \simeq 0$, then $E_1 - E_2 \simeq 2|H_{1,2}|$. If the unperturbed energy levels were degenerated, then the perturbed energy levels will not remain so. The removal of the degeneracy is called *level repulsion*.

We can illustrate this phenomena by considering an arbitrary 2×2 hermitian matrix and computing its eigenvalues.

$$H = \begin{pmatrix} H_{1,1} & H_{1,2} \\ H_{1,2}^* & H_{2,2} \end{pmatrix}$$

The eigenvalues will be given by eq. (1.3).

The first case, $|H_{1,2}| \ll \delta$, can be viewed as the case when the off-diagonal elements are small and the matrix can be approximated with a diagonal matrix. In this case we expect that the energy levels will be close to the diagonal levels or the unperturbed levels. The perturbed eigenstates will also be approximatively equal with the unperturbed eigenstates.

The level repulsion emphasised by the second case, $|H_{1,2}| \gg \delta$, corresponds to the case when the off-diagonal elements are significant. When we expand the perturbed eigenstates in the basis given by the unperturbed eigenstates we will have significant components from each element in the basis and the new states will be a mixture of the unperturbed states. We can say that the energy levels are no longer independent. In the case when the unperturbed energy levels are degenerated, the difference between the perturbed energy levels is given by $2|H_{1,2}|$, which is a measure of the mixing of the unperturbed states.

1.4 Probability notions

Definition (Joint probability). Given two events A and B , their joint probability, $P(A \cap B)$, is the probability of the two events to occur simultaneously.

Definition (Conditional probability). The conditional probability of an event A given an event B with $P(B) > 0$, denoted $P(A|B)$ is given by

$$P(A|B) = \frac{P(A \cap B)}{P(B)}.$$

The joint probability of A and B can be expressed as $P(A \cap B) = P(A|B)P(B)$.

Definition (Continuous random variable). A continuous random variable is a function from the set of all outcomes to the set of real numbers $X : \Omega \rightarrow (R)$ such that

$$P(a \leq X(\omega) \leq b) = \int_a^b f(x) dx,$$

where $f(x) \geq 0$ and $\int_{-\infty}^{+\infty} f(x) dx = 1$.

The above function f is called the *probability density function*. The probability for a continuous random variable X to take a value in the infinitesimal interval of length dx is given by

$$P(x \in [x, x + dx]) = \int_x^{x+dx} f(z) dz \approx f(x) dx \quad (1.4)$$

1.5 Nearest neighbour distributions

Nearest neighbour spacing distributions show how the differences between consecutive energy levels fluctuate around the average. In order to better understand this concept we shall begin with the simpler case of real random numbers as presented in [5] and then continue with a general case as in [6].

1.5.1 The nearest neighbour spacing distribution of random numbers

We consider a sequence of uniformly distributed, ordered, real, random numbers. We define the *spacing* of an ordered sequence as the sequence of differences between consecutive elements. For an interval of length s , $s > 0$, we will denote with $P(n \in s)$ the probability for the interval to contain n numbers and with $P(n \in ds | m \in s)$ the conditional probability for the interval of length ds to contain n numbers given that the interval of length s contains m numbers.

If E is a given number in the sequence, we are interested in the probability $P(s)ds$ to have the next number between $E + s$ and $E + s + ds$. Since we are interested in the next number after E , we know that in the interval of length s there is no other number and the next number is somewhere in the infinitesimal interval ds . Thus the joint probability of the events $1 \in ds$ and $0 \in s$ is given by:

$$P(s) ds = P(1 \in ds | 0 \in s) P(0 \in s). \quad (1.5)$$

Since random numbers are not correlated, the probability of a random number to be found in the interval ds does not depend on the number of random numbers in s , so

$$P(1 \in ds | 0 \in s) = P(1 \in ds).$$

The random numbers are uniformly distributed, so their probability density function f is a constant. Hence, according to eq. (1.4), the probability of finding a number in the interval of length ds is given by

$$P(1 \in ds) \equiv P(1 \in [0, 0 + ds]) \approx f(s) ds \sim ds.$$

If we denote the constant probability density function with a

$$P(s) ds = a ds P(0 \in s).$$

$P(0 \in s)$ can be expressed using the complementary probability as $1 - \int_0^s P(s') ds'$. Now we can express $P(s) ds$ as follows:

$$P(s) ds = a ds \left(1 - \int_0^s P(s') ds' \right).$$

In order to differentiate with respect to s , we will use the Leibniz rule for differentiating integrals, namely

$$\frac{d}{dx} \int_{G(x)}^{H(x)} F(x, t) dt = \int_{G(x)}^{H(x)} \frac{\partial F}{\partial x} dt + F(x, H(x)) \frac{dH}{dx} - F(x, G(x)) \frac{dG}{dx} \quad (1.6)$$

Using this rule, we obtain

$$\frac{d}{ds} P(s) = -a P(s).$$

This differential equation can be solved by separation of variables, yielding

$$P(s) = \mathcal{C} e^{-as}$$

In order to determine the constant \mathcal{C} , we use the normalisation condition for the probability density function

$$\int_{-\infty}^{\infty} P(s) ds = 1$$

Since $s > 0$, this reduces to

$$\int_0^{\infty} P(s) ds = \int_0^{\infty} \mathcal{C} e^{-as} ds = -\frac{\mathcal{C}}{a} e^{-as} \Big|_0^{\infty} = \frac{\mathcal{C}}{a}$$

Thus $\mathcal{C} = a$ and $P(s) = a e^{-as}$. We can further simplify the formula if we set that the average spacing to unity. The average spacing is given by

$$\bar{s} = \int_0^{\infty} s P(s) ds = - \int_0^{\infty} s \frac{d}{ds} (e^{-as}) ds = \int_0^{\infty} e^{-as} ds = \frac{1}{a},$$

so setting it to unity results in $a = 1$. Thus the probability density function becomes

$$P(s) = e^{-s}. \quad (1.7)$$

This function is known as the *Poisson distribution*.

1.5.2 The Wigner distribution

We will now consider a more complicated situation, by considering the probability density function for the sequence of random numbers to be arbitrary.

We can start from eq. (1.5) since the discussion up to that point did not include any details related to the distribution of the random numbers.

In this case $P(1 \in ds | 0 \in s) = f_{1,0}(s) ds$, where $f_{n,m}(s)$ is function which describes how the probability of having n numbers in ds is influenced by the m numbers in s . Thus

$$P(s) ds = f_{1,0}(s) ds \left(1 - \int_0^s P(s') ds' \right)$$

By solving this integral equation, we obtain the solution

$$P(s) = \mathcal{C} f_{1,0}(s) \exp \left(- \int_0^s f_{1,0}(x) dx \right)$$

We observe that if we take the probability density function constant, $f_{1,0}(s) = \frac{1}{a}$, we obtain the above case of the Poisson distribution. For a probability density function, $f_{1,0}(s) = \alpha s$ we obtain

$$P(s) = \mathcal{C} \alpha s \exp \left(-\alpha \frac{s^2}{2} \right)$$

From the normalisation condition we obtain

$$\int_0^\infty P(s) \, ds = \mathcal{C} = 1$$

The average spacing is given by

$$\bar{s} = \int_0^\infty s P(s) \, ds = \alpha \int_0^\infty s^2 \exp\left(-\alpha \frac{s^2}{2}\right) \, ds = \frac{1}{\sqrt{\alpha}} \sqrt{\frac{\pi}{2}}.$$

If we set the average spacing to unity, we obtain $\alpha = \frac{\pi}{2}$ and

$$P(s) = \frac{\pi}{2} s \exp\left(-\frac{\pi}{4} s^2\right)$$

This function is known as the *Wigner distribution*.

1.6 From Classical Chaos to Quantum Chaos

The classical concept of sensitivity to initial conditions loses its meaning in the quantum realm since the trajectory cannot be defined due to Heisenberg's uncertainty principle. However, there are some other ways in which we can link classically chaotic dynamics to quantum features. These bridges between classical mechanics and quantum mechanics allows us to give a meaning to quantum chaos [7].

Specifically, there are two important conjectures that allow us to connect classical systems and quantum systems as mentioned above.

The Berry-Tabor conjecture

This conjecture states that the quantum counterpart of a classically integrable system has a Poissonian nearest neighbour distribution.

The Bohigas-Gianoni-Schmit conjecture

This conjecture states that the nearest neighbour distribution of a quantum system with a classically chaotic counterpart is given by the Wigner distribution.