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Fingerprints of classical phase space structure in quantum chaos

Bachelor Thesis

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Chapter 1

Introduction

Chapter 2

Classical chaos

2.1 Fundamental notions

Classical mechanics can be reformulated in a more elegant way which does not require the computation of individual forces and instead uses a single function to describe the entire system, namely the *Lagrangian*. The Lagrangian is a function of the generalised coordinates $q_1, \ldots, q_n$, their derivatives with respect to time $\dot{q_1}, \ldots, \dot{q_n}$ and optionally the time t, where n is the number of degrees of freedom.

The principles of Newtonian mechanics are replaced by the a variational principle $\delta S = 0$, where

$$S = \int_{t_1}^{t_2} \mathcal{L}\, \mathrm{d}t \tag{2.1}$$

is called the *action*. This principle, also called *Hamilton's principle* or *the principle of least action* is equivalent with the Euler-Lagrange equations

$$\frac{\partial \mathcal{L}}{\partial q_k} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathcal{L}}{\partial \dot{q_k}} = 0,$$

where $k = 1, \ldots, n$. Thus we have n second order differential equations.

An other formalism for classical mechanics which is very useful in theoretical physics is the Hamiltonian formalism. In this formalism instead of the Lagrangian we use the *Hamiltonian*, which is a function of the generalised coordinates $q_1, \ldots, q_n$, the generalised momenta $p_1, \ldots, p_n$ and optionally the time t. The generalised momenta is given by

$$p_k = \frac{\partial \mathcal{L}}{\partial \dot{q_k}}.$$

The Hamiltonian can be obtained from the Lagrangian through a *Legendre*

transformation of $\mathcal{L}$

$$\mathcal{H}(q_1, \ldots, q_n, p_1, \ldots, p_n, t) = \sum_{k=0}^{n} p_k \dot{q}_k - \mathcal{L}(q_1, \ldots, q_n, \dot{q}_1, \ldots, \dot{q}_n, t). \tag{2.2}$$

The Euler-Lagrange equations are replaced by Hamilton's equations

$$\dot{q}_k = \frac{\partial \mathcal{H}}{\partial p_k}$$
$$\dot{p}_k = -\frac{\partial \mathcal{H}}{\partial q_k}$$

We now have $2n$ first order ordinary differential equations. comments?

2.2 Canonical transformations

In the Hamiltonian formulation of classical mechanics *canonical transformations* represent all the transformations of the canonically conjugate variables from q and p to Q and P such that the structure of the Hamilton equations remains intact.

The Lagrange equations of a system are invariant to a transformation of the Lagrange function such that:

$$\mathcal{L}'(Q, \dot{Q}, t) = \mathcal{L}(q, \dot{q}, t) - \frac{\mathrm{d}}{\mathrm{d}t} F(q, Q, t)$$

Integrating we obtain

$$\int_{t_1}^{t_2} \mathcal{L}' \, \mathrm{d}t = \int_{t_1}^{t_2} \mathcal{L} \, \mathrm{d}t - (F(q, Q, t_2) - F(q, Q, t_1))$$

The variation of the above equation is given by

$$\delta \int_{t_1}^{t_2} \mathcal{L}' \, \mathrm{d}t = \delta \int_{t_1}^{t_2} \mathcal{L} \, \mathrm{d}t - \delta F(q, Q, t_2) + \delta F(q, Q, t_1)$$

Fixing the variations at the end points to be 0, we get

$$\delta \int_{t_1}^{t_2} \mathcal{L}' \, \mathrm{d}t = \delta \int_{t_1}^{t_2} \mathcal{L} \, \mathrm{d}t$$

So indeed the two Lagrangian descriptions of the system are identical since if the Hamilton principle holds in the first description it also holds in the second.

A function $F(q, Q, t)$ satisfying the above property and the condition $\frac{\partial^2 F}{\partial q \partial Q} \neq 0$ is called a *generating function*. We can classify the generating functions in four

possible types as a function of their variables. The conjugate momenta corresponding to q and Q are given by

$$p = \frac{\partial \mathcal{L}}{\partial \dot{q}} \text{ and } P = \frac{\partial \mathcal{L}'}{\partial \dot{Q}}$$

In order to express those as a function of $F(q, Q, t)$ we use the fact that $\dot{q}$ is a cyclic coordinate for $\mathcal{L}'$

$$\frac{\partial \mathcal{L}'}{\partial \dot{q}} = \frac{\partial \mathcal{L}}{\partial \dot{q}} - \frac{\partial}{\partial \dot{q}} \left(\frac{\mathrm{d}}{\mathrm{d}t} F(q, Q, t) \right) = \frac{\partial \mathcal{L}}{\partial \dot{q}} - \frac{\partial F}{\partial q} = 0,$$

where

$$\frac{\mathrm{d}}{\mathrm{d}t} F(q, Q, t) = \frac{\partial F}{\partial q} \dot{q} + \frac{\partial F}{\partial Q} \dot{Q} + \frac{\partial F}{\partial t}.$$

Thus we obtain

$$p = \frac{\partial \mathcal{L}}{\partial \dot{q}} = \frac{\partial F}{\partial q}$$

and

$$P = \frac{\partial \mathcal{L}'}{\partial \dot{Q}} = -\frac{\partial F}{\partial Q}$$

To find the Hamiltonian corresponding to the new coordinates Q and P we compute the Legendre transformation of $\mathcal{L}'$

$$\mathcal{H}'(Q, P, t) = P\dot{Q} - \mathcal{L}'(Q, \dot{Q}, t)$$

Thus

$$\mathcal{H}'(Q, P, t) = P\dot{Q} - \mathcal{L} + \frac{\mathrm{d}F}{\mathrm{d}t} = P\dot{Q} - \mathcal{L} + \frac{\partial F}{\partial q} \dot{q} + \frac{\partial F}{\partial Q} \dot{Q} + \frac{\partial F}{\partial t} = p\dot{q} - \mathcal{L} + \frac{\partial F}{\partial t}$$

and so

$$\mathcal{H}'(Q, P, t) = \mathcal{H}(q(Q, P), p(Q, P), t) + \frac{\partial F(q(Q, P), Q, t)}{\partial t}. \tag{2.3}$$

As mentioned above, there are four types of generating functions. They can be obtained by successive Legendre transformations which switch between the conjugate coordinates and they represent the same canonical transformation. We denote the above mentioned $F(q, Q, t) \equiv F_1(q, Q, t)$. The other types of generating

functions will be denoted $F_2(q,P,t), F_3(p,Q,t), F_4(p,P,t)$. Thus we define

$$\begin{aligned} F_2(q,P,t) &= F_1(q,Q,t) + PQ \\ p &= \frac{\partial F_2}{\partial q}, \quad Q = \frac{\partial F_2}{\partial P} \\ F_3(p,Q,t) &= F_1(q,Q,t) - pq \\ q &= -\frac{\partial F_3}{\partial p}, \quad P = \frac{\partial F_3}{\partial Q} \\ F_4(p,P,t) &= F_1(q,Q,t) - pq + PQ \\ q &= -\frac{\partial F_4}{\partial p}, \quad Q = \frac{\partial F_4}{\partial P} \end{aligned}$$

The *Poisson bracket* of two arbitrary functions with respect to the canonical coordinates q and p is defined as

$$[F,G]_{q,p} = \sum_{k=1}^{n} \left(\frac{\partial F}{\partial q_k}\frac{\partial G}{\partial p_k} - \frac{\partial F}{\partial p_k}\frac{\partial G}{\partial q_k} \right)$$

As with the above discussion we will limit to the case of one degree of freedom, but the results are easily generalisable to n degrees of freedom.

If Q and P are a set of conjugate variables obtained by a canonical transformation from q and p, then

$$[F',G']_{Q,P} = [F,G]_{q,p},$$

where F' and G' are the transformed functions. Proof? As a consequence, if we choose $F = Q$ and $G = P$

$$[Q,P]_{Q,P} = [Q(q,p), P(q,p)]_{q,p} = 1$$

This relation represents a necessary and sufficient condition for the transformation from q,p to Q,P to be canonical and is equivalent with the definition given for the canonical transformations.

An other equivalent condition would require the Jacobian matrix $\frac{\partial(Q,P)}{\partial(q,p)}$ to be that symplectic.

2.3 The Hamilton-Jacobi equation

Instead of finding the equations of motion through solving a set of $2n$ ordinary differential equations with $2n$ dependent variables ($q_1,\ldots,q_n$ and $p_1,\ldots,p_n$) and one independent variable (t), we can use a single first order partial differential

equation having $n+1$ independent variables ($q_1, \ldots, q_n$ and t) and one dependent variable (S).

Suppose there exists a generating function S of type F_2 why? such that

$$\mathcal{H}' = 0.$$

From Hamilton's equations, the new coordinates Q_k and P_k, with $k = 1, \ldots, n$ will be constants, so the information about the time evolution of the system is contained in the canonical transformation itself.Thus, equation (2.3) becomes

$$\mathcal{H}(q_1, \ldots, q_n, \frac{\partial S}{\partial q_1}, \ldots, \frac{\partial S}{\partial q_n}, t) + \frac{\partial S}{\partial t} = 0 \tag{2.4}$$

which represents the *Hamilton-Jacobi equation.*

The solution $S(q_1, \ldots, q_n, P_1, \ldots, P_n, t)$ of equation (2.4) is called *Hamilton's Principal Function.* From the theory of differential equations we know that there will be $n+1$ arbitrary constants. We can find n of these constants as $P_1, \ldots, P_n$ and the remaining constant can be incorporated in S since if S is a solution for the Hamilton-Jacobi equation, $S + const.$ is also a solution.

It is a standard convention (Goldstein) to rename the constants as follows

$$\begin{aligned} P_k &\equiv \alpha_k \\ Q_k \equiv \beta_k &= \frac{\partial S(q_1, \ldots, q_n, \alpha_1, \ldots, \alpha_n, t)}{\partial \alpha_k}. \end{aligned}$$

These constants depend on the initial conditions $q_k(0)$ and $p_k(0)$. From

$$p_k(0) = \left.\frac{\partial S(q_1, \ldots, q_n, \alpha_1, \ldots, \alpha_n, t)}{\partial q_k}\right|_{t=0}$$

we can obtain α_ks, and β_ks are given by

$$\beta_k = \left.\frac{\partial S(q_1, \ldots, q_n, \alpha_1, \ldots, \alpha_n, t)}{\partial \alpha_k}\right|_{t=0}$$

We can obtain the initial generalised coordinates $q_k(\alpha_1, \ldots, \alpha_n, \beta_1, \ldots, \beta_n, t)$ by solving

$$\beta_k = \frac{\partial S}{\partial \alpha_k}$$

If we take the total time derivative of S

$$\frac{\mathrm{d}S}{\mathrm{d}t} = \sum_{k=0}^{n} \frac{\partial S}{\partial q_k}\dot{q}_k + \frac{\partial S}{\partial t}$$

and use eq. (2.3)

$$\frac{\mathrm{d}S}{\mathrm{d}t} = \sum_{k=0}^{n} p_k \dot{q}_k - \mathcal{H}$$

we recognise the Legendre transform from eq. (2.2). Thus

$$\frac{\mathrm{d}S}{\mathrm{d}t} = \mathcal{L}$$

or equivalently

$$S = \int \mathcal{L}\,\mathrm{d}t\,.$$

It follows that the generating function for this special canonical transformation is the action as defined in eq. (2.1).

If the time does not appear explicitly in the Hamiltonian, the Hamiltonian itself will be a constant of the motion and will represent the energy of the system E.

We can rewrite eq. (2.4) as follows

$$\mathcal{H}(q_1, \ldots, q_n, \frac{\partial S}{\partial q_1}, \ldots, \frac{\partial S}{\partial q_n}, t) = -\frac{\partial S}{\partial t} = E$$

Thus we can suppose that for this case $S(q_1, \ldots, q_n, \alpha_1, \ldots, \alpha_n, t)$ has the following form

$$S(q_1, \ldots, q_n, \alpha_1, \ldots, \alpha_n, t) \equiv W(q_1, \ldots, q_n, \alpha_1, \ldots, \alpha_n) - Et$$

Using this expression in eq. (2.4), we obtain

$$\mathcal{H}(q_1, \ldots, q_n, \frac{\partial W}{\partial q_1}, \ldots, \frac{\partial W}{\partial q_n}) = E \tag{2.5}$$

which represents the second form of the Hamilton-Jacobi equation.

The solution to this equation is called *Hamilton's Characteristic Function*. W can be expressed as

$$W = S + Et = \int (\mathcal{L} + \mathcal{H})\,\mathrm{d}t = \int \sum_{k=0}^{n} p_k \dot{q}_k\,\mathrm{d}t = \sum_{k=0}^{n} \int p_k\,\mathrm{d}q_k$$

physical interpretation?

W is a generating function of type F_2. The canonical transformation given by W is different from the one given by S, since $\mathcal{H}' = \mathcal{H} + \frac{\partial W}{\partial t} = E \neq 0$.

The new generalised coordinates Q_k are cyclic in the new Hamiltonian $\mathcal{H}' = E = \mathcal{H}(q_1, \ldots, q_n, \frac{\partial W}{\partial q_1}, \ldots, \frac{\partial W}{\partial q_n})$, thus the new generalised momenta care constants. While in the case of S all the generalised momenta and coordinates were constants,

in the case of W all the generalised momenta are constants $\dot{P}_k = -\frac{\partial \mathcal{H}'}{\partial Q_k} = 0$, but not all the generalised coordinates are constants. If we choose to define $P_1 \equiv E$,

$$\dot{Q}_1 = \frac{\partial \mathcal{H}'}{\partial P_1} = \frac{\partial E}{\partial P_1} = 1$$

Thus

$$Q_1 = t + const. = \frac{\partial W}{\partial P_1} = \frac{\partial W}{\partial E}.$$

So Q_1 is no longer a constant. The constant in the above equation determines the origin of the time axis. Q_1 represents the time and its conjugate coordinate is P_1, the energy.

The $n-1$ generalised momenta $P_2, \ldots, P_n$ are independent of P_1 and thus $\frac{\partial \mathcal{H}'}{\partial P_k} = 0$, where $k = 2, \ldots, n$. So the corresponding $n-1$ generalised coordinates are constants.

We can change the notation for α and β to use an index from 1 to $n-1$: $\alpha_j \equiv P_{j+1}$, $\beta_j \equiv Q_{j+1}$, where $j = 1, \ldots, n-1$. We can now express Hamilton's Characteristic Function as

$$W = W(q_1, \ldots, q_n, E, \alpha_1, \ldots, \alpha_{n-1}).$$

From the initial generalised momenta $p_k(0)$

$$p_k(0) = \left. \frac{\partial W(q_1, \ldots, q_n, E, \alpha_1, \ldots, \alpha_{n-1})}{\partial q_k} \right|_{t=0}$$

we can obtain E and α_j. Using the initial generalised coordinates $q_k(0)$ we obtain β_j as follows

$$\beta_j = \left. \frac{\partial W(q_1, \ldots, q_n, E, \alpha_1, \ldots, \alpha_{n-1})}{\partial \alpha_j} \right|_{t=0}$$

Thus, having E, α_j and β_j, we can obtain the time evolution for the generalised coordinates from

$$\beta_j = \frac{\partial W(q_1, \ldots, q_n, E, \alpha_1, \ldots, \alpha_{n-1})}{\partial \alpha_j}$$

For systems with $n > 1$ degrees of freedom, the Hamilton-Jacobi equation can be separated in n equations if we can write S as

$$S(q_1, \ldots, q_n, \alpha_1, \ldots, \alpha_n, t) = \sum_{k=1}^{n} W_k(q_k, \alpha_1, \ldots, \alpha_n) - Et$$

A simpler form of separability exists if the Hamiltonian itself is separable

$$\mathcal{H}(q_1, \ldots, q_n, p_1, \ldots, p_n) = \sum_{k=1}^{n} \mathcal{H}_k(q_k, p_k)$$

In this case the second form of the Hamilton-Jacobi equation splits in n independent equations

$$\mathcal{H}(q_1, \ldots, q_n, p_1, \ldots, p_n) = E = \sum_{k=1}^{n} \mathcal{H}_k(q_k, p_k),$$

so

$$\mathcal{H}_k(q_k, \frac{\partial W_k}{\partial q_k}) = \alpha_k, \qquad E = \sum_{k=1}^{n} \alpha_k$$

why $E = \sum_{k=1}^{n} \alpha_k$?

The Hamilton-Jacobi equation can be solved only in some situations (only when the variables can be separated. why?), depending both on the problem and the chosen coordinate system. For orthogonal coordinates the *Staeckel conditions* (see Goldstein pp. 453) establish which kind of potentials can be separated. This does not decrease the theoretical value of the Hamilton-Jacobi equation which provides powerful methods for finding the constants of the motion.

2.4 Action-angle variables

Going back again to a system with one degree of freedom for simplicity, we study a system which has a periodic motion. We search for a canonical transformation from q, p to a new set of canonically conjugate coordinates θ, I such that the new Hamiltonian does not depend on θ.

Since θ is an ignorable coordinate

$$\dot{I} = -\frac{\partial \mathcal{H}'}{\partial \theta} = 0,$$

I is a constant of the motion and

$$\dot{\theta} = \frac{\partial \mathcal{H}'}{\partial I} = const.$$

Thus $\theta = \frac{\partial \mathcal{H}'}{\partial I}(t - t_0) \equiv \omega(I)(t - t_0)$. θ is called the *angle variable* and I the *action variable* (not to be confused with the action).

In order to obtain this variables we will use a generating function of type F_1 denoted $W'(q, \theta)$. Since the motion is periodic in the initial coordinates, it must also be periodic in the angle variable. Thus W' is periodic in θ.

From the properties of the F_1 type generating functions

$$\mathrm{d}W' = \frac{\partial W'}{\partial q}\,\mathrm{d}q + \frac{\partial W'}{\partial \theta}\,\mathrm{d}\theta = p\,\mathrm{d}q - I\,\mathrm{d}\theta\,.$$

(we can observe that W' is related to Hamilton's Characteristic Function by a Legendre transformation)

Since the motion is periodic, if we integrate over a period q returns to the same value, while θ advances by a constant amount, which we can choose to be 2π per period.

$$\oint \mathrm{d}W' = 0 = \oint p\,\mathrm{d}q - \oint I\,\mathrm{d}\theta$$

Since I is a constant of the motion,

$$2\pi I = \oint p\,\mathrm{d}q$$

or

$$I = \frac{1}{2\pi}\oint p\,\mathrm{d}q\,. \tag{2.6}$$

Equation (2.6) can be considered the definition for the action variable, where the integral is taken around a single period of the motion (which is always a closed curve in phase space).

2.5 Integrability

A system called *integrable* if the number of degrees of freedom is equal to the number of constants of the motion in involution which each other. Two constants of the motion are in *involution* with each other if their mutual Poisson brackets are equal to 1.

The previously mentioned constants of the motion are not required to be known in analytic form, they are only required to exist. Thus, for example $n = 1$ systems are always integrable if the Hamiltonian is time independent.

For integrable systems, the n constants of the motion restrict the motion in the $2n$ dimensional phase space to a $2n - n = n$ dimensional subspace. If the motion is also periodic, then the motion is constrained to a n dimensional closed surface (with finite volume).

For a system with $n = 2$ and periodic motion, the motion in the phase space is confined to a torus. In order to understand why, we can use the previously defined action-angle variables. In this case, the motion will be described by $I_1, \theta_1, I_2, \theta_2$. Since the motion is constrained to a 2 dimensional subspace, we can imagine the phase space as a plane with the Ox axis given by the direction in which θ_1 increases and with the Oy axis given by the direction in which θ_2 increases. Because the motion is periodic, we can consider that θ_i, $i = 1, 2$ takes values in $[0, 2\pi)$. Since the values for 0 and 2π are equivalent, we can join the ends of the intervals in both directions, thus forming a torus.

To extend the discussion to systems with n degrees of freedom, we replace the 2D plane with an n dimensional cube. If we join the sides of this cube we obtain a n dimensional torus.

Connection with the "hairy ball" theorem

we consider a vector field associated with the tangent in each point of the trajectory in phase space. This vector field is generated by Hamilton's equations with time as parameter(why?/how?). In the $n = 2$ case we can see that if the the shape of the closed bi-dimensional surface were a sphere, we could not "comb" the vectors without creating a singularity. Instead, if the surface is a torus, the problem disappears. This result is a consequence of the "hairy ball" theorem. This theorem states that there is no non-vanishing continuous tangent vector field on even-dimensional n-spheres. (what happens for odd n?)

+ explanation for the fact that the constants of motion must be in involution with each other

2.6 Chaos notions

2.7 Kolmogorov-Arnol'd-Moser theorem

Chapter 3

Quantum Chaos

3.1 Random matrix theory

3.1.1 Nearest neighbour spacing distributions

Nearest neighbour spacing distributions show how the differences between consecutive energy levels fluctuate around the average.

We consider a sequence of uniformly distributed, ordered, real, random numbers. Let E represent a number in the sequence. The probability $P(s)\,\mathrm{d}s$ to have the next number between $E+s$ and $E+s+\mathrm{d}s$ is given by:

$$P(s)\,\mathrm{d}s = P(1 \in \mathrm{d}s \,|\, 0 \in s)P(0 \in s),$$

where $P(n \in s)$ represents the probability for s to contain n numbers and $P(n \in \mathrm{d}s \,|\, m \in s)$ is the *conditioned* probability for the interval of length $\mathrm{d}s$ to contain n numbers when the interval of length s contains m numbers.

Since random numbers are not correlated, the probability of a random number to be found in the interval $\mathrm{d}s$ does not depend on the number of random numbers in s, so

$$P(1 \in \mathrm{d}s \,|\, 0 \in s) = P(1 \in \mathrm{d}s).$$

Since the random numbers are uniformly distributed, the probability (density?) of finding a number in the interval $\mathrm{d}s$ is constant. We denote this constant with a. Thus

$$P(s)\,\mathrm{d}s = a\,\mathrm{d}sP(0 \in s).$$

$P(0 \in s)$ can be expressed using the complementary probability as $1 - \int_s^\infty P(s')\,\mathrm{d}s'$. Now we can express $P(s)\,\mathrm{d}s$ as follows:

$$P(s)\,\mathrm{d}s = a\,\mathrm{d}s\left(1 - \int_s^\infty P(s')\,\mathrm{d}s'\right).$$

Using the Leibniz rule for differentiating integrals,

$$\frac{\mathrm{d}}{\mathrm{d}x}\int_{G(x)}^{H(x)} F(x,t)\,\mathrm{d}t = \int_{G(x)}^{H(x)} \frac{\partial F}{\partial x}\,\mathrm{d}t + F(x,H(x))\,\frac{\mathrm{d}H}{\mathrm{d}x} - F(x,G(x))\,\frac{\mathrm{d}G}{\mathrm{d}x}$$

we obtain

$$\frac{\mathrm{d}}{\mathrm{d}s}P(s) = -aP(s)$$

when differentiating with respect to s.

Chapter 4

Procedure

4.1 The Hamiltonian

In this chapter we will describe how we obtained the numerical results. We begin by computing the matrix elements of the Hamiltonian in a basis given by the eigenstates of an isotropic double harmonic oscillator. In analogy with the classical case, we consider two independent quantum numbers n_1, n_2 corresponding to the two orthogonal oscillating directions. We can define two number operators N_1, N_2 such that $N_1 |n_1, n_2\rangle = n_1 |n_1, n_2\rangle$ and $N_2 |n_1, n_2\rangle = n_2 |n_1, n_2\rangle$. We consider the creation and annihilation operators $a_1^\dagger, a_1$ and $a_2^\dagger, a_2$ such that $N_1 = a_1^\dagger a_1$ and $N_2 = a_2^\dagger a_2$. In terms of the previously defined operators, the Hamiltonian of the isotropic double harmonic oscillator is given by

$$H_0 = \hbar\omega_0 \left(a_1^\dagger a_1 + \frac{1}{2} I + a_2^\dagger a_2 + \frac{1}{2} I \right) = \hbar\omega_0 \left(N_1 + N_2 + I \right)$$

and its eigenstates are given by

$$H_0 |n_1, n_2\rangle = \hbar\omega_0 \left(n_1 + n_2 + 1 \right) |n_1, n_2\rangle$$

Since $n_1 + n_2 = n$ can be obtained in $\sum_{i=0}^{n} i = \frac{1}{2} n(n+1)$ ways, the energy levels of the isotropic double harmonic oscillator are $\frac{1}{2} n(n+1)$ fold degenerated.

In the fundamental state $|0, 0\rangle$, with $n_1 = n_2 = 0$, the oscillator has the energy equal to $\hbar\omega_0$, having a *zero point motion* (details / definition?). Since we are interested (why?) in variations from the equilibrium state, we can rescale the potential energy such that the energy of the fundamental state becomes 0. Thus the new Hamiltonian will be given by

$$H_0 = A \left(N_1 + N_2 \right),$$

where $A = \hbar\omega_0$.

We can construct the basis starting from the vacuum state $|0,0\rangle$ by acting with the creation operators

$$a_1^{\dagger n_1}|0,0\rangle = \sqrt{n_1!}\,|n_1,0\rangle$$
$$a_2^{\dagger n_2}|0,0\rangle = \sqrt{n_2!}\,|0,n_2\rangle$$

Thus, by applying the operator $a_1^{\dagger n_1}a_2^{\dagger n_2}$ such that $n_1+n_2=n$ (in order to obtain for each n all the states with the energy $n\,\hbar\omega_0$ wrt vacuum) we obtain the basis elements ordered as follows:

$$|0,0\rangle\,|0,1\rangle\,|0,2\rangle\cdots|0,n\rangle\,|1,0\rangle\,|1,1\rangle\cdots|1,n-1\rangle\cdots|i,0\rangle\,|i,1\rangle\cdots|i,n-i\rangle\cdots|n,0\rangle\,.$$

For our investigations, the Hamiltonian is expressed as a function of the creation and annihilation operators up to fourth order terms as follows

$$\begin{aligned}
H = A\left(a_1^\dagger a_1 + a_2^\dagger a_2\right) + \frac{B}{4}\Big[&\left(3a_1^\dagger a_2^{\dagger 2} + 3a_1 a_2^2 - a_1^{\dagger 3} - a_1^3\right)\\
&+ 3\left(a_1 a_2^{\dagger 2} + a_1^\dagger a_2^2 - a_1^\dagger a_1^2 - a_1^{\dagger 2}a_1 + 2a_1 a_2^\dagger a_2 + 2a_1^\dagger a_2^\dagger a_2\right)\Big]\\
+ \frac{D}{16}\Big[&6\left(a_1^{\dagger 2}a_1^2 + a_2^{\dagger 2}a_2^2\right) + 2\left(a_1^2 a_2^{\dagger 2} + a_1^{\dagger 2}a_2^2\right) + 8a_1^\dagger a_1 a_2^\dagger a_2\\
&+ 4\left(a_1^\dagger a_1^3 + a_1^{\dagger 3}a_1 + a_2^\dagger a_2^3 + a_2^{\dagger 3}a_2 + a_1^2 a_2^\dagger a_2 + a_1^{\dagger 2}a_2^\dagger a_2 + a_1^\dagger a_1 a_2^2 + a_1^\dagger a_1 a_2^{\dagger 2}\right)\\
&+ \left(a_1^{\dagger 4} + a_1^4 + a_2^{\dagger 4} + a_2^4 + 2a_1^{\dagger 2}a_2^{\dagger 2} + 2a_1^2 a_2^2\right)\Big].
\end{aligned} \tag{4.1}$$

The physical origin of this Hamiltonian is related to quadrupole vibrations of nuclear surfaces. (details for B, D?) (add citations) The energy levels will be expressed in units of harmonic oscillator energy and therefore from here on we will consider $A=1$. We can obtain the eigenvalues and eigenvectors of the Hamiltonian by a diagonalization routine based on Relatively Robust Representations from Intel® Math Kernel Library used via a `Python` program(+ citations). Any such diagonalization method requires a truncation of the Hilbert space which induces errors concerning the eigenvalues. This errors increase as one moves to the upper limit of the energy for a fixed dimension of the Hilbert space. Indeed we expect this energies to have more important contributions from the states that were eliminated by truncation. We tested the stability of the energy levels by comparing the results obtained for different sizes of the diagonalization basis as is detailed in the next section.

4.2 Stability

We consider the *stable levels* to be the eigenvalues which, at a change of basis from one with a dimension of N to one with dimension $N + \Delta N$, do not change with more than a chosen threshold δ_s. In the following figure we show the variation of the energy levels when the dimension increases from $N = 120$ to $N = 140$.

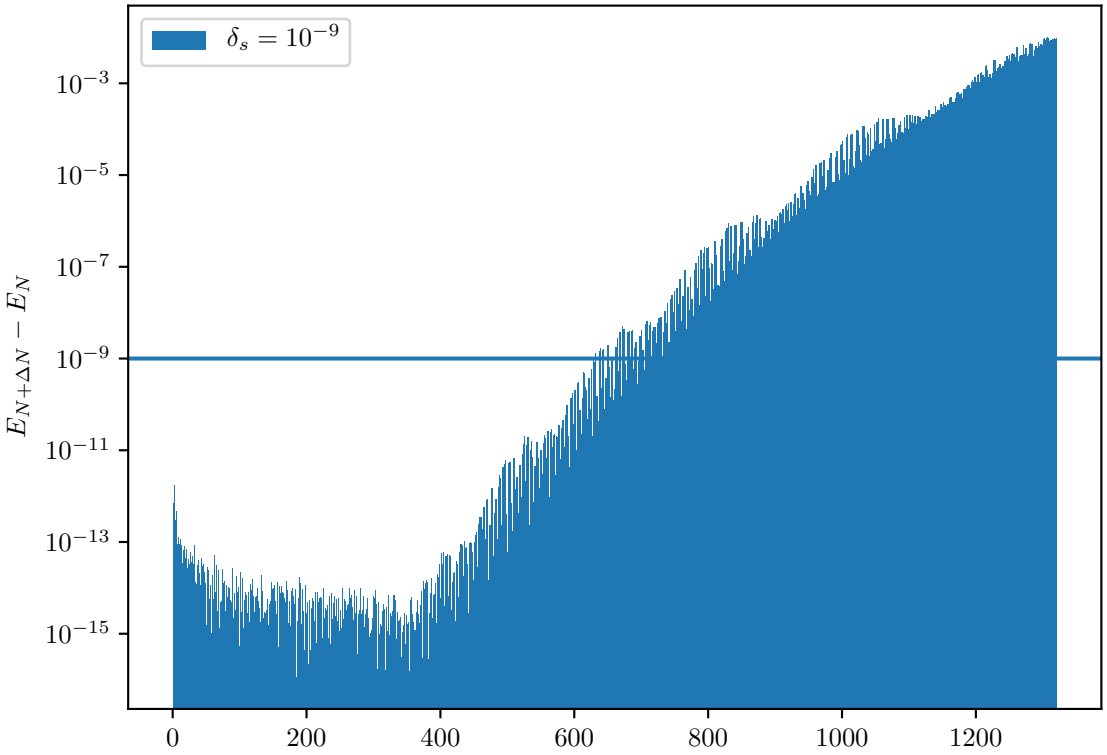


Figure 4.1: $B = 0.2, D = 0.4, N = 120$

We can observe that the first 400–600 eigenvalues have a very good stability. Thus we can choose the stability threshold for example at $\delta_s = 10^{-9}$. Qualitatively the shape of this distribution does not depend on the parameters of the Hamiltonian or the dimension of the Hilbert space because it reflects the nature of the approximation as discussed previously. For example, for $B = 0.55, D = 0.4, N = 260$ compared with $N = 280$

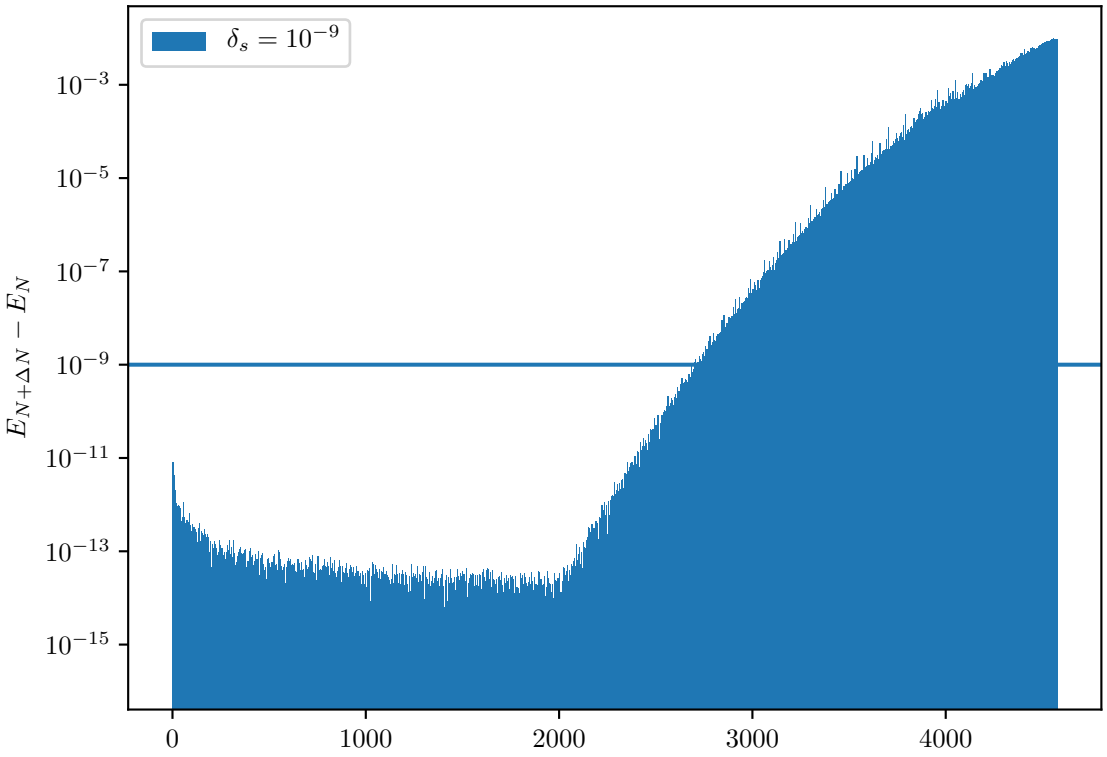


Figure 4.2: $B = 0.55, D = 0.4, N = 260$

As expected, the number of stable levels increases with the size of the basis. Roughly, for a given basis size N, the first 7–8% levels differ with less than $\delta_s = 10^{-9}$ when we compare with a basis of dimension $N + \Delta N$, with $\Delta N = 20$.

4.3 Statistics

As we mentioned in the Introduction, a spectrum can be characterised through the probability distribution of the nearest neighbour spacing. The *spacing* is defined as the difference between two consecutive energy levels. Similarly the *relative spacing* is defined as

$$s = \frac{E_{i+1} - E_i}{\overline{\Delta E}},$$

where $\overline{\Delta E}$ is the average spacing $\frac{E_n - E_0}{N}$.

The *nearest neighbour spacing distributions* tell us the probability $P(s)\,\mathrm{d}s$ to find a relative spacing s when we move in the spectrum obtained by diagonalization. This probability is defined as follows

$$P(s)\,\mathrm{d}s = \frac{N_{s,s+\Delta s}}{N},$$

where $N_{s,s+\Delta s}$ is the number of levels with the relative spacing between s and $s + \Delta s$. We can also define a *cumulative probability distribution*,

$$I(s) = \sum_{s_i=0}^{s} P(s_i)\Delta s$$

4.3.1 Irreducible representations

In order to analyse the fluctuations of the previously obtained eigenvalues we must first take into account the symmetry of the system. The symmetries of a system can make influence the fluctuations making the given sequence of levels appear more regular than it actually is (better explanation & citation). In order to remove this influence we analyse separately each symmetry reduced subspace or equivalently each *irreducible representation* of the Hamiltonian.

If an operator A corresponds to a symmetry of the Hamiltonian, then it commutes with the Hamiltonian, $[A, H] = 0$. (Proof?) For the Hamiltonian in eq. (4.1) we have the following symmetries (?), which correspond to the symmetry group $\mathcal{C}_{3v}$. This group has 3 irreducible representations: one bi-dimensional and two unidimensional, namely (notation?).

Separating the bi-dimensional representation

The presence of the bi-dimensional representation corresponds a two-fold degeneracy which allows us to identify it by computing the differences between consecutive levels $\Delta E = E_{i+1} - E_i$. An other option is to use directly the relative spacing, which differs only by a constant from ΔE, namely the average spacing. The separation of the symmetric and anti-symmetric irreducible representations will be detailed later.

In figure 4.3 we can see how ΔE varies with the index of the levels.

Because of the finite precision of the numerical implementation, the difference between two consecutive degenerate levels might not be exactly 0, its value depending on the machine precision (as it can be seen in the above figure). To take this fact into account we will consider that the levels which have s (or ΔE) greater than a chosen ε belong to one of the unidimensional representations. In order to choose a suitable value for ε, we use a histogram to visualise the number of levels at different spacings (see figure 4.4a).

This bimodal shape of the histogram suggests clearly the presence of the degenerate levels well separated from the rest. For some particular values for B (such as $B = 0.4$) and high values for N ($N > 200$), we observed a splitting of the block corresponding to the degenerated levels in two blocks, namely one at exactly 0 and the other at low values. (see fig. 4.4b)

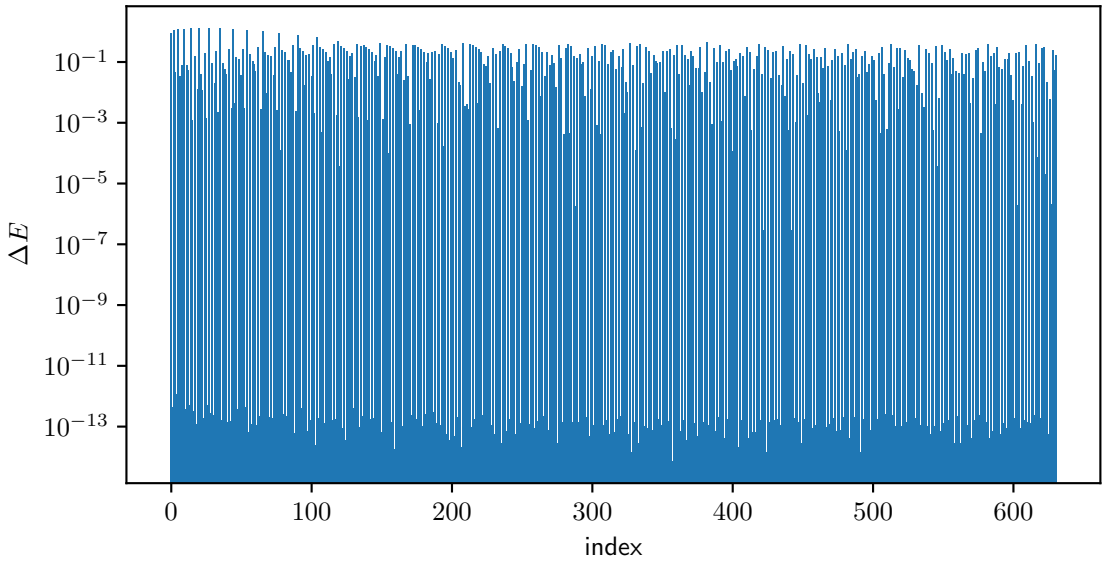
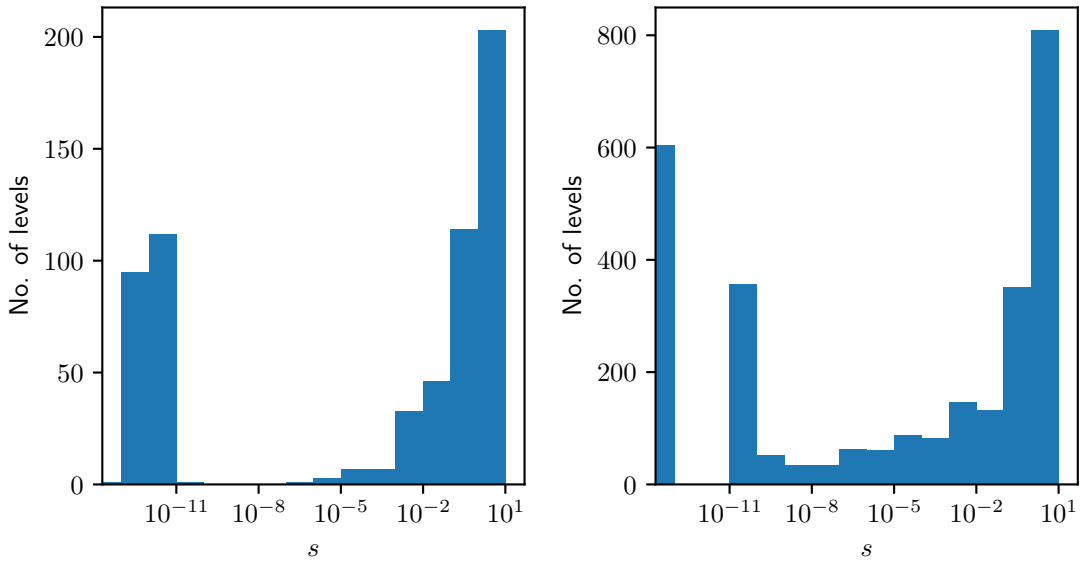


Figure 4.3: $B = 0.2, D = 0.4, N = 120$



(a) $B = 0.2, D = 0.4, N = 120$ (b) $B = 0.4, D = 0.4, N = 260$

Figure 4.4: The relative spacing histograms for different parameters

If we plot the spacing as a function of the level index, we can see how each level is situated with respect to the chosen ε. Once again we can observe how the spacings corresponding to the bi-dimensional representation are separated from the rest.

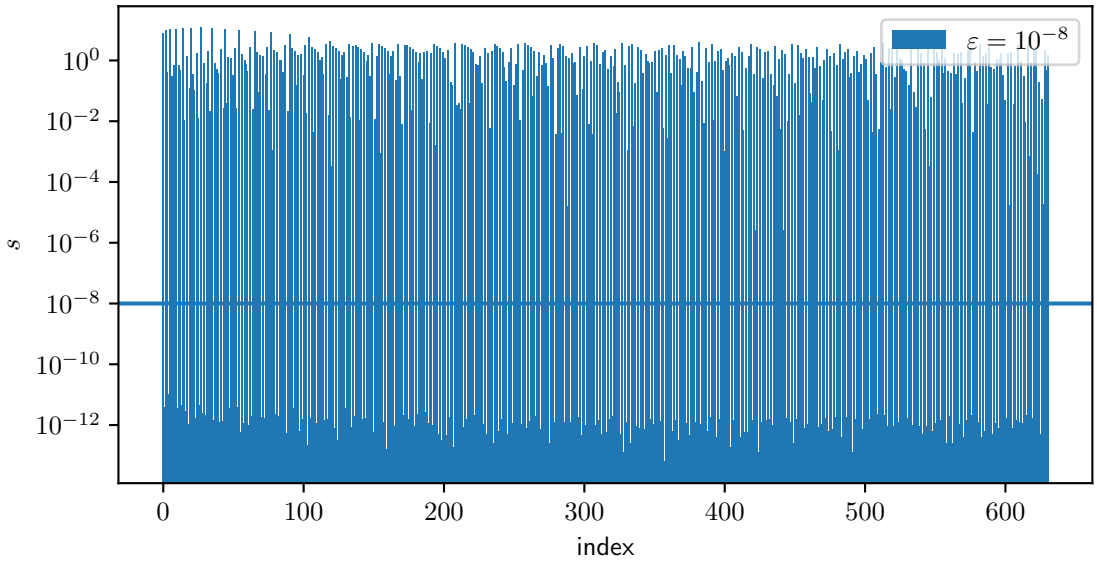


Figure 4.5: $B = 0.2, D = 0.4, N = 120$

Separating the unidimensional representations

In order to identify the unidimensional representations we rely on the symmetry of the potential energy operator,

…?

We can observe that this operator is invariant to a reflection along the Ox? axis. axis $\rightarrow$ n_2? For the harmonic oscillator the states with even quantum numbers have even wave functions. (proof / cite?) Thus, we can establish a correspondence (how?) between the symmetry of the representation and the parity of the quantum number n_2 such that the unidimensional symmetric representation corresponds to an even n_2 and the unidimensional anti-symmetric representation corresponds to an odd n_2.

The values of the quantum numbers n_1 and n_2 depend on the ordering of the basis. Because the diagonalisation algorithm returns the eigenvalues (and the corresponding eigenvectors) in ascending order, the initial ordering of the basis is lost. One method to approximate n_1 and n_2 for a given eigenvector would be to consider that their values are given by the index of the dominant coefficient.

Thus, if we have the following eigenvector

$$\begin{pmatrix} C_{0,0} \\ C_{0,1} \\ \vdots \\ C_{0,n} \\ C_{1,0} \\ \vdots \\ C_{1,n-1} \\ \vdots \\ C_{i,0} \\ \vdots \\ C_{i,n-i} \\ \vdots \\ C_{n,0} \end{pmatrix}$$

and $C_{i,j}$ is the greatest coefficient, than we assign to this eigenvector the quantum numbers of the k-th element in the basis, where k is the index of the coefficient.

For example, for the simplified case of the isotropic double harmonic oscillator ($B = D = 0$) with $N = 3$, the Hamiltonian is given by

$$H = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 \end{pmatrix}$$

The eigenvalues will be $E_i = 0, 1, 1, 2, 2, 2$ with the corresponding eigenvectors

$$v_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \; v_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \; v_3 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \; v_4 = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \; v_5 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \; v_6 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

Since the basis is given by

$$|0,0\rangle \, |0,1\rangle \, |0,2\rangle \, |1,0\rangle \, |1,1\rangle \, |2,0\rangle \, ,$$

the quantum numbers for the eigenvectors will be assigned as follows

$$
\begin{aligned}
v_1 &\equiv |0,0\rangle \text{ since } k = 1 \\
v_2 &\equiv |0,1\rangle \text{ since } k = 2 \\
v_3 &\equiv |1,0\rangle \text{ since } k = 4 \\
v_4 &\equiv |0,2\rangle \text{ since } k = 3 \\
v_5 &\equiv |2,0\rangle \text{ since } k = 6 \\
v_6 &\equiv |1,1\rangle \text{ since } k = 5
\end{aligned}
$$

Maximum is not unique?

...

In figures 4.6 and 4.7 we can see the relative spacing for each irreducible representation as a function of index and as a histogram.

We can plot the average spacing as a function of B (see fig. 4.10) (details?) Selection problems?

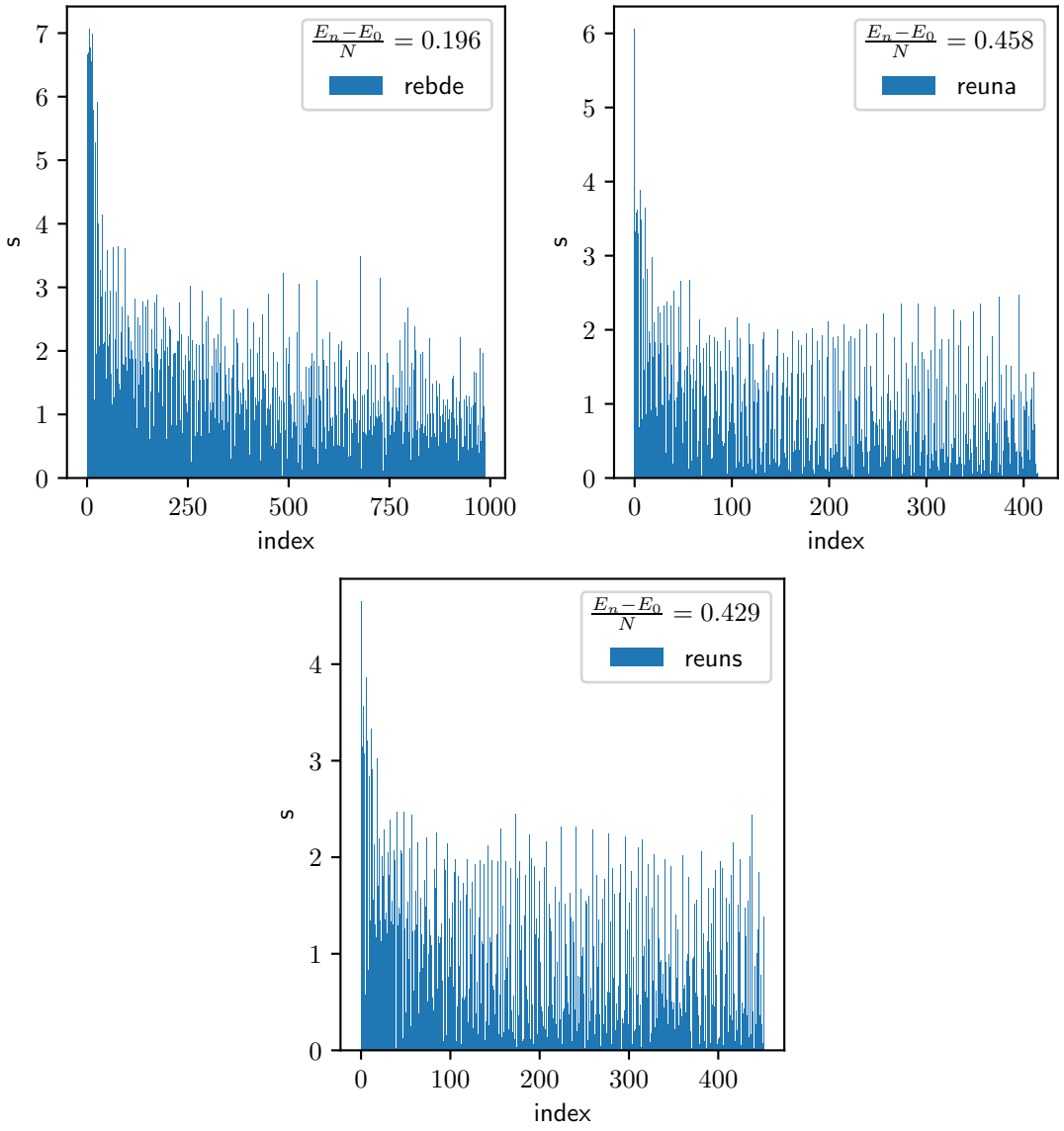


Figure 4.6: The relative spacing for each irreducible representation as a function of index for $B = 0.2, D = 0.4, N = 260$

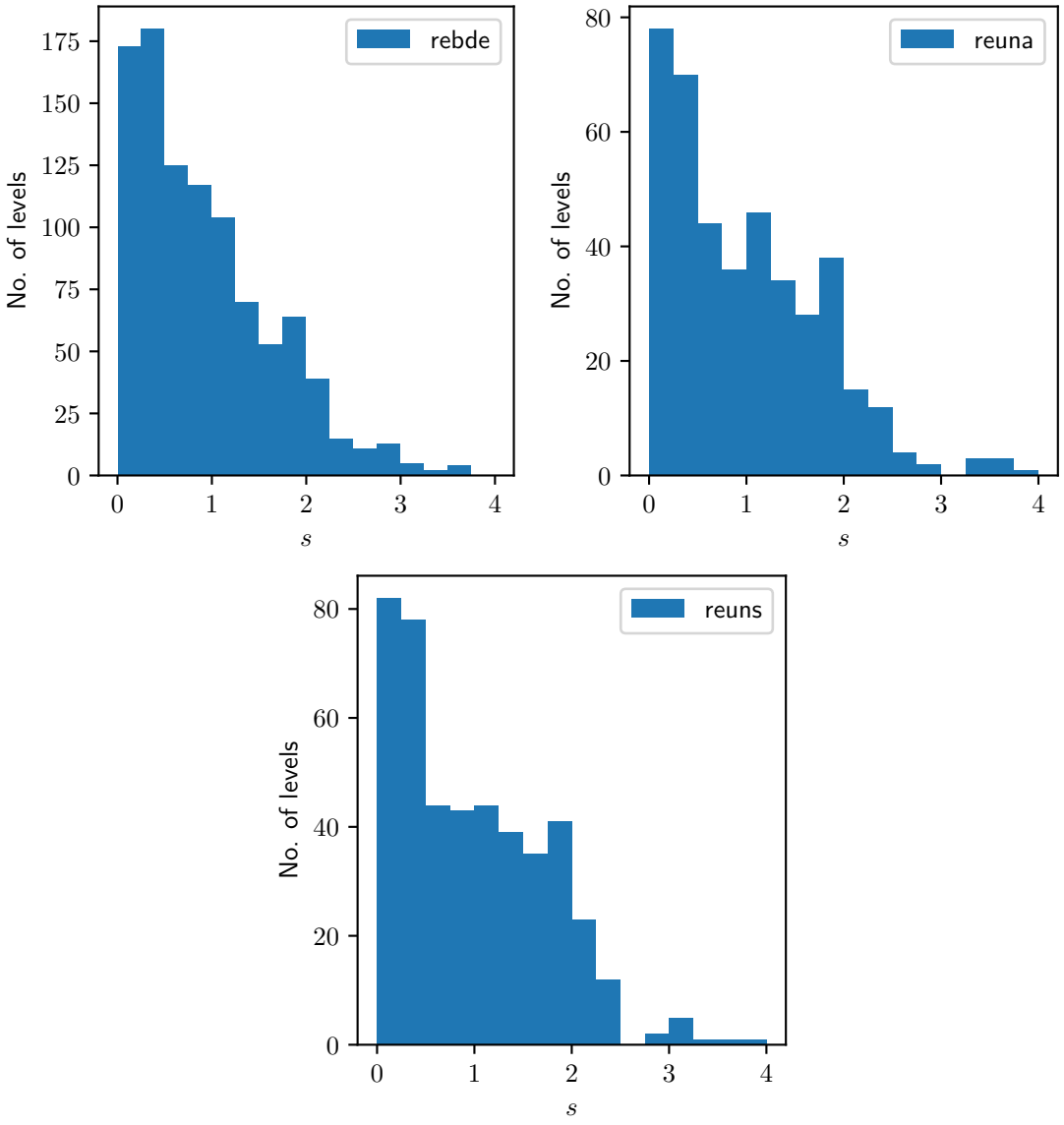


Figure 4.7: The relative spacing histogram for each irreducible representation for $B = 0.2, D = 0.4, N = 260$

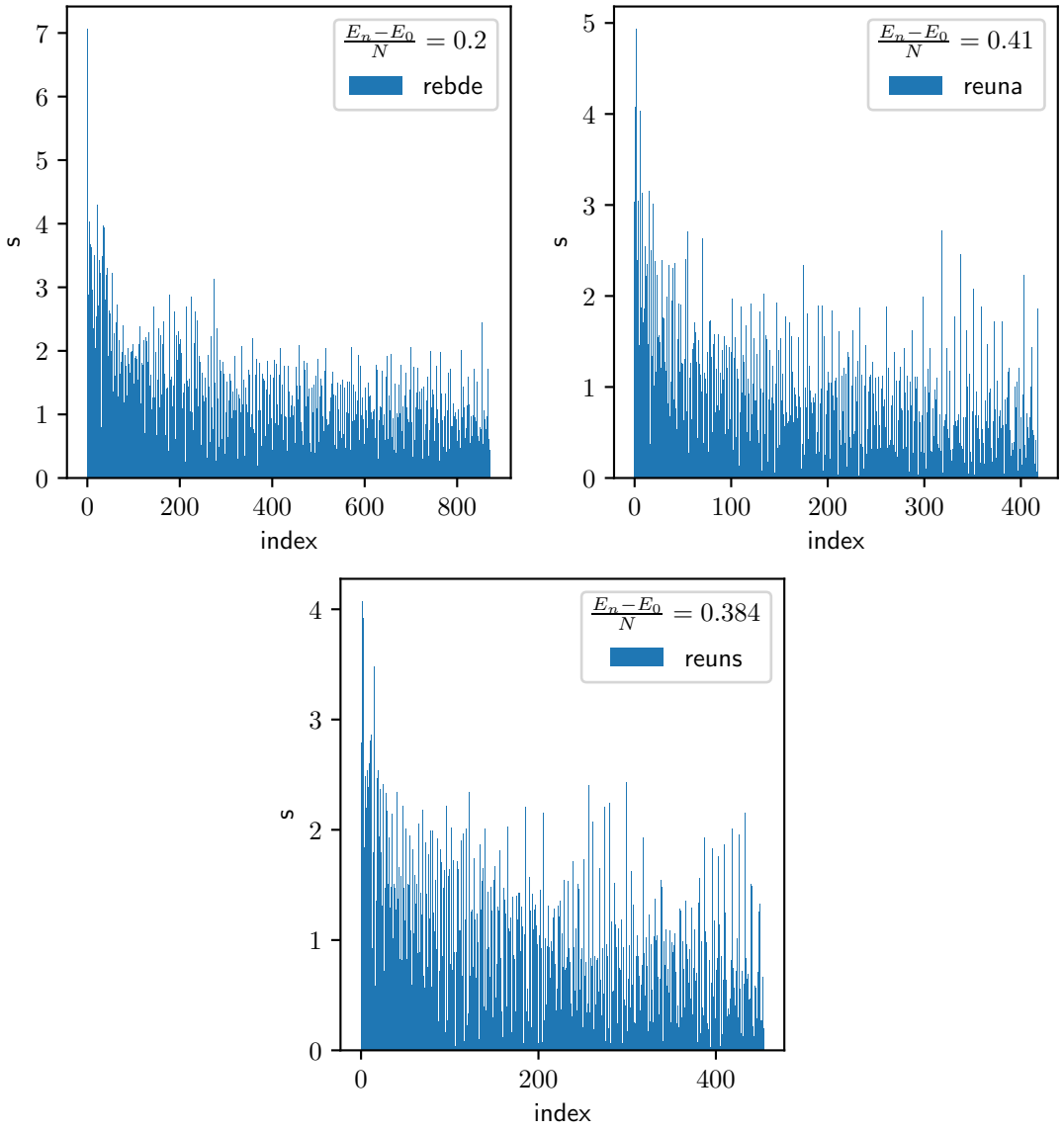


Figure 4.8: The relative spacing for each irreducible representation as a function of index for $B = 0.63, D = 0.4, N = 260$

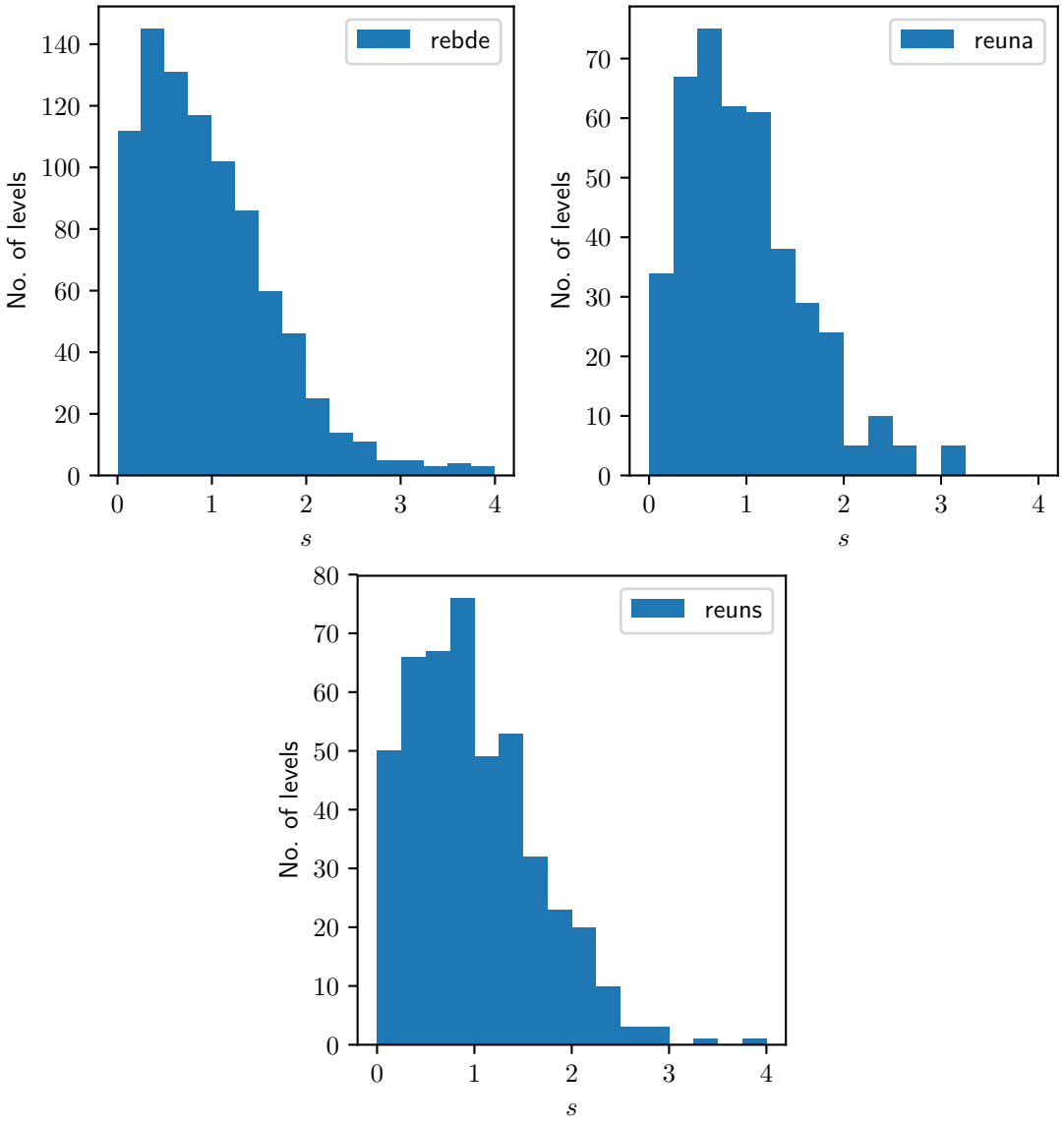


Figure 4.9: The relative spacing histogram for each irreducible representation for $B = 0.63, D = 0.4, N = 260$

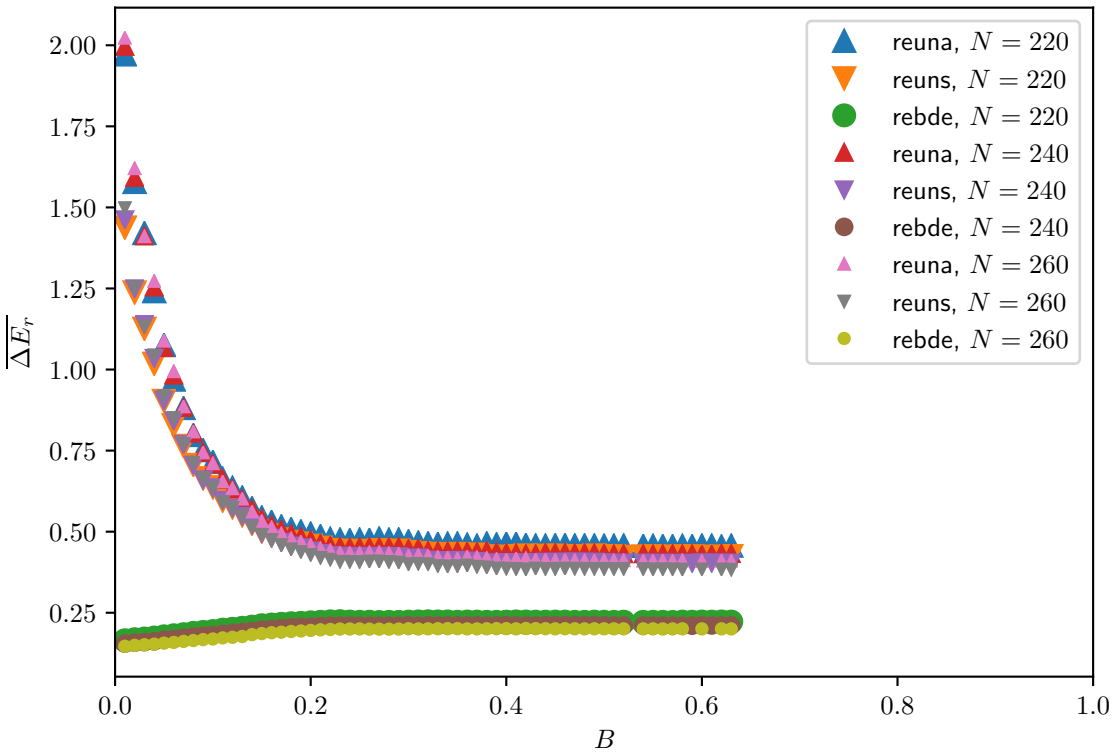


Figure 4.10: $\overline{\Delta E}$ as a function of B for each representation

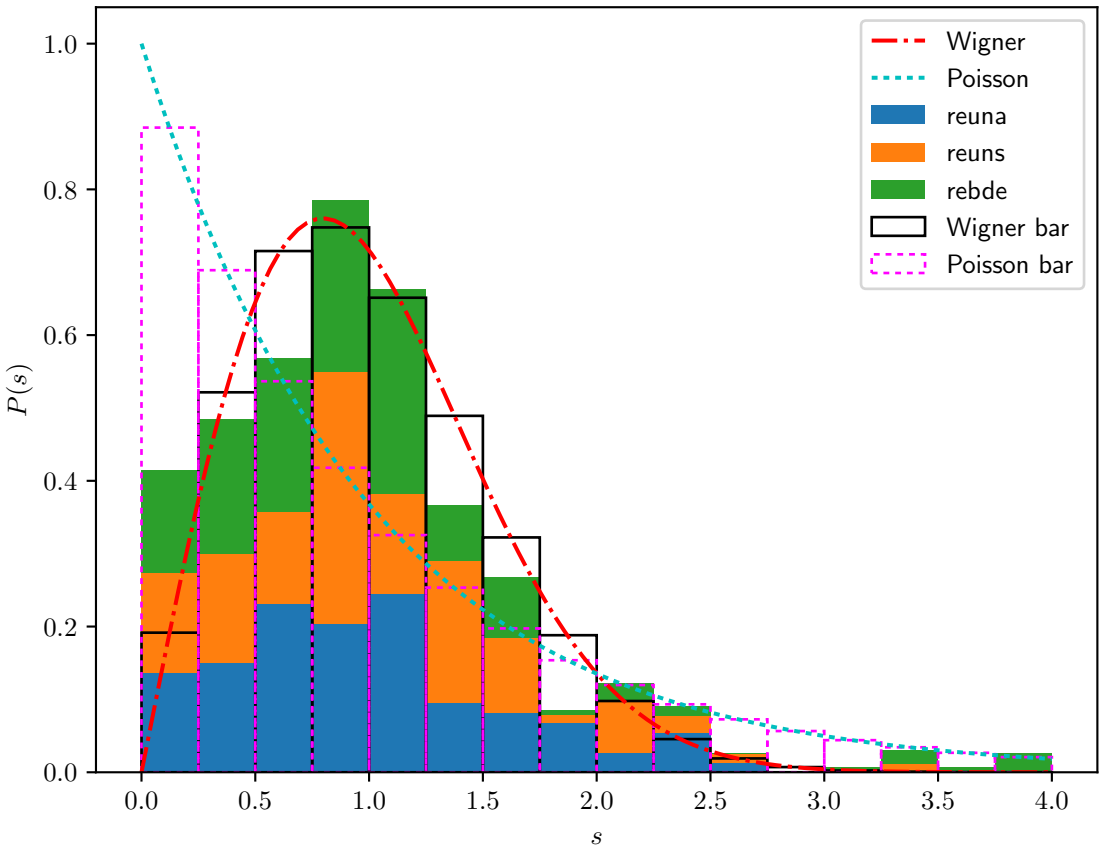


Figure 4.11: $B = 0.2, D = 0.4, N = 120$

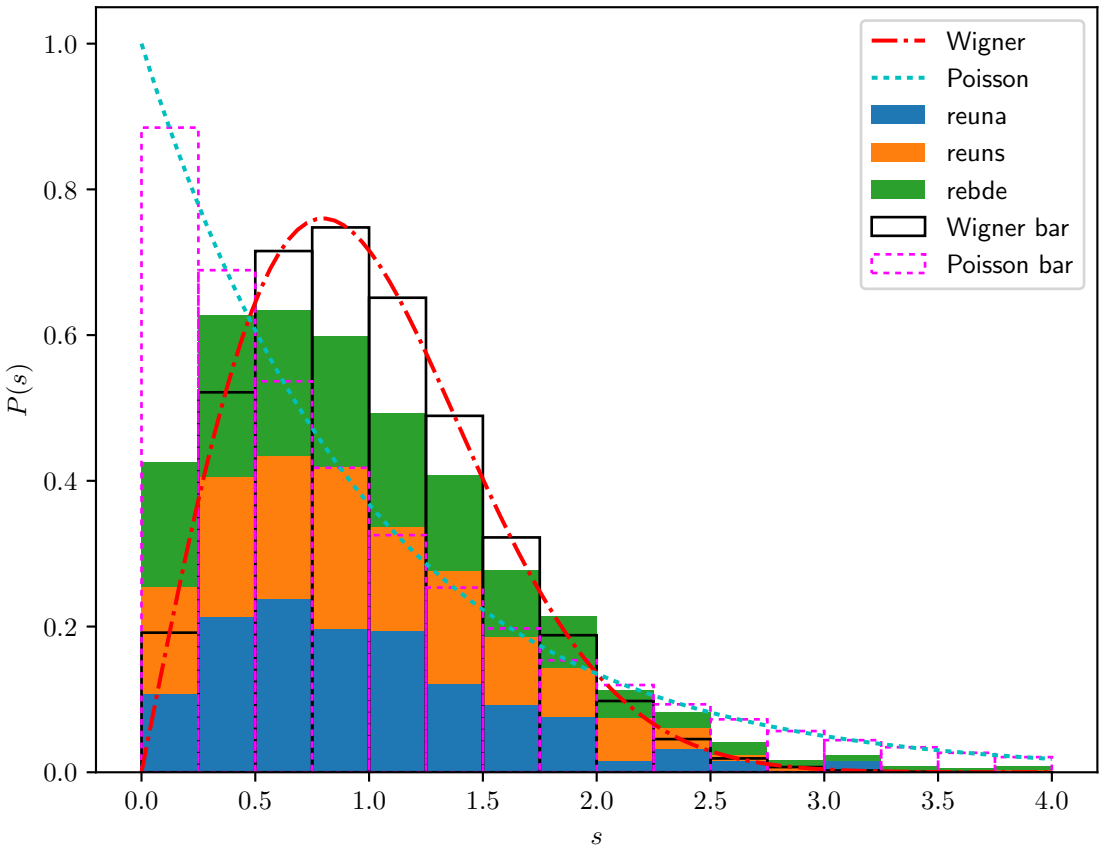


Figure 4.12: $B = 0.63, D = 0.4, N = 260$

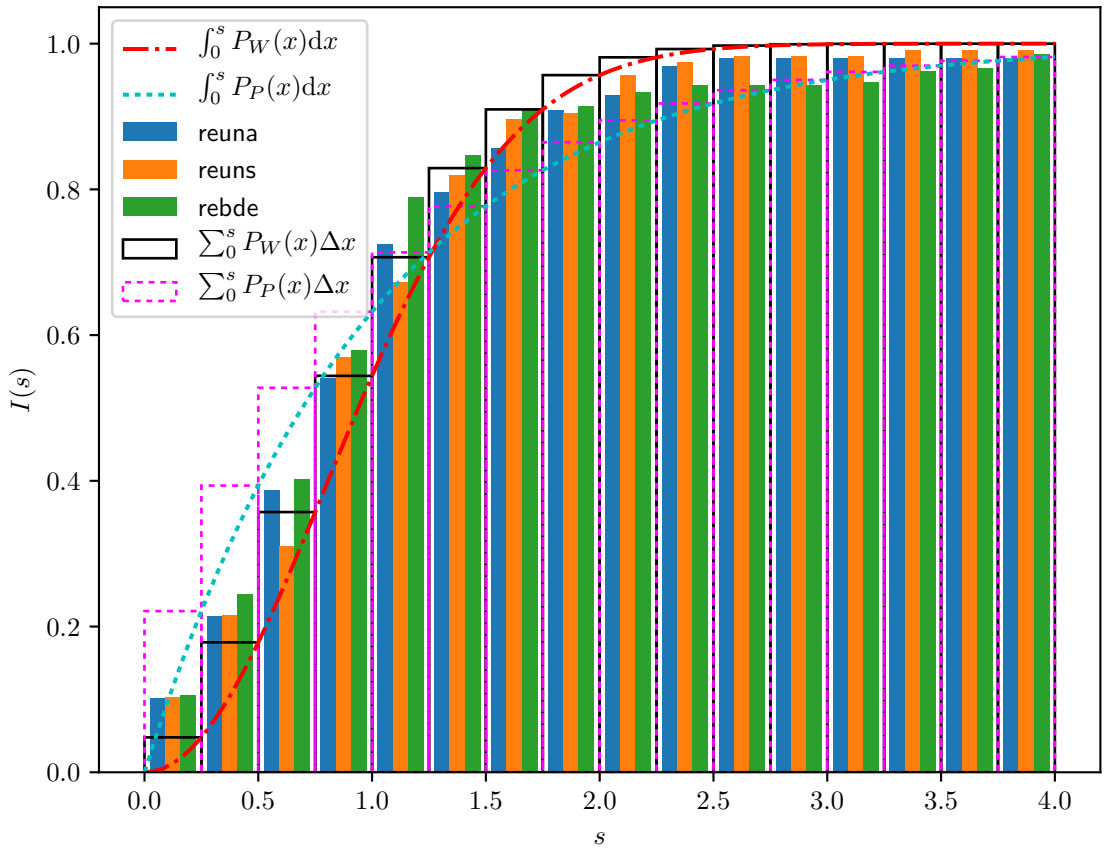


Figure 4.13: $B = 0.2, D = 0.4, N = 120$

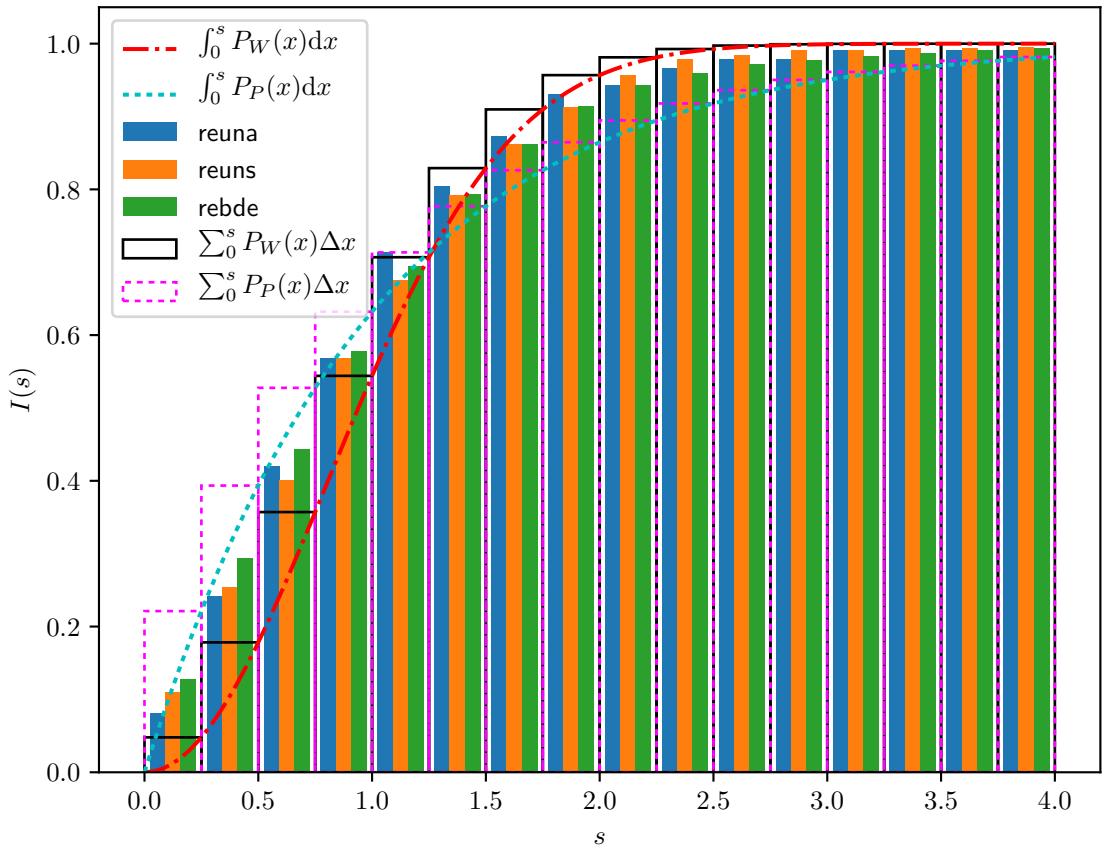


Figure 4.14: $B = 0.63, D = 0.4, N = 260$

Chapter 5

Results

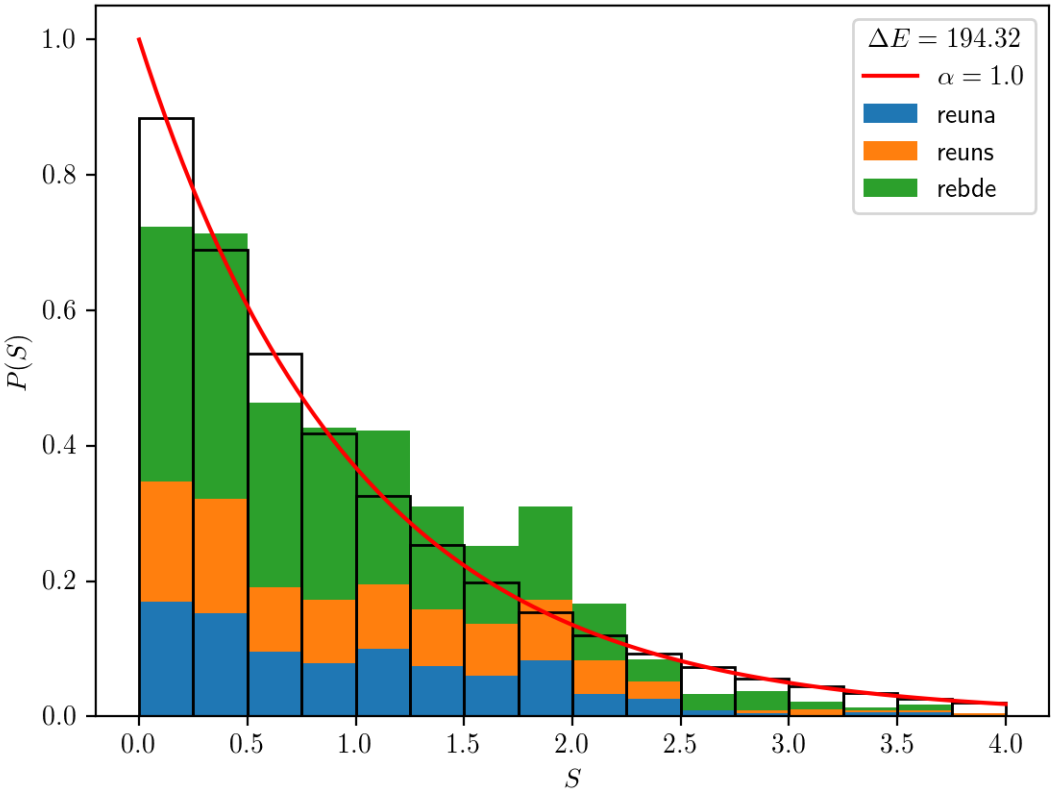


Figure 5.1: $B = 0.2, D = 0.4, N = 260$

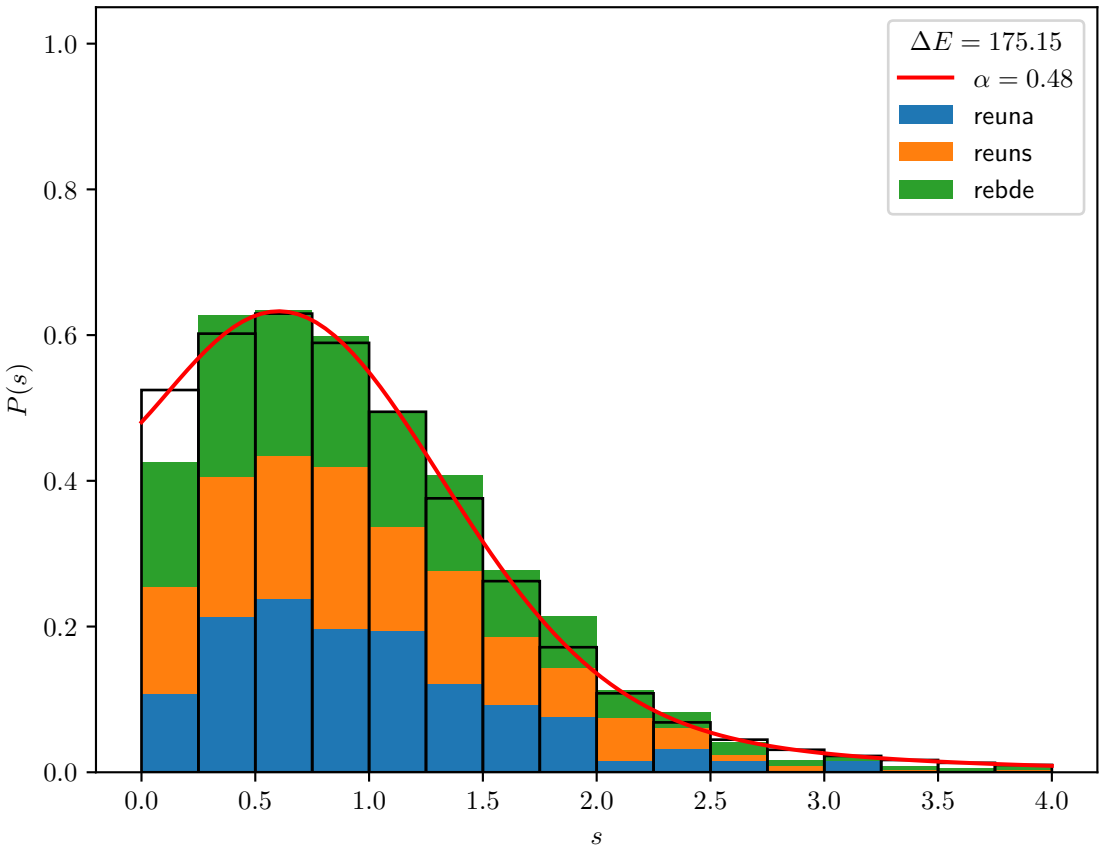


Figure 5.2: $B = 0.63, D = 0.4, N = 260$

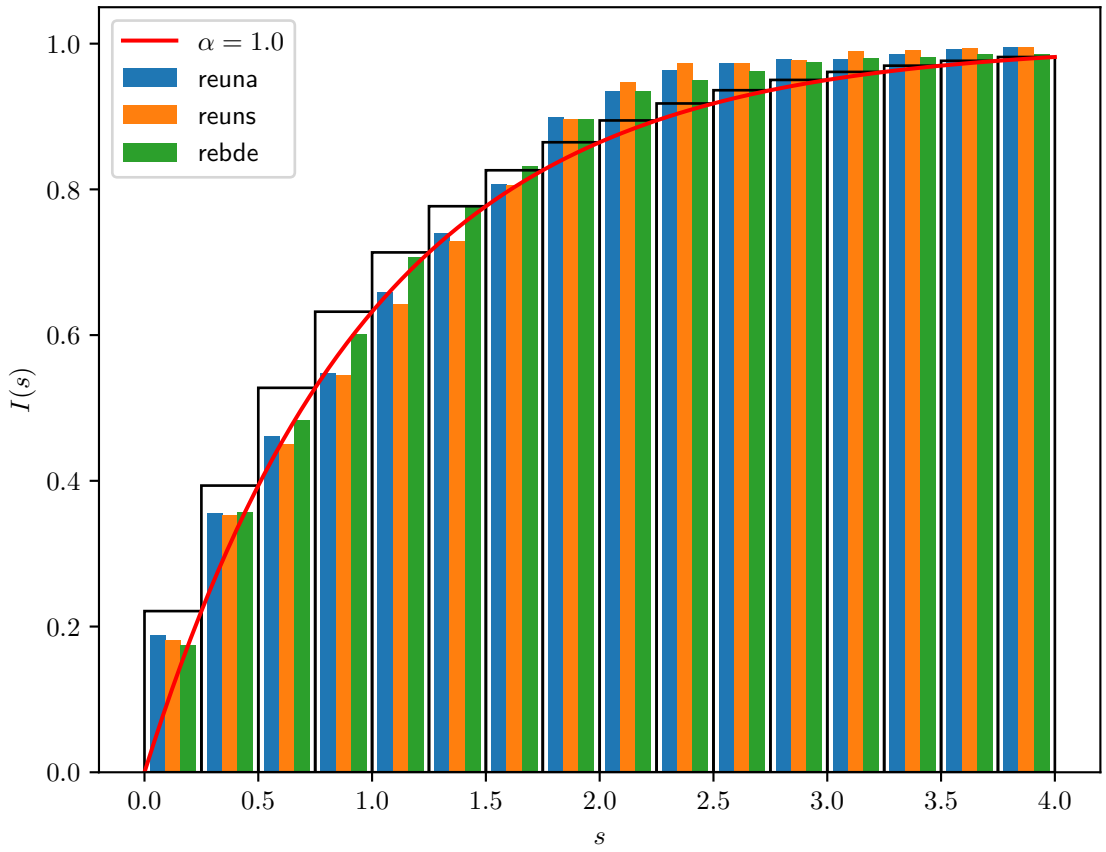


Figure 5.3: $B = 0.2, D = 0.4, N = 260$

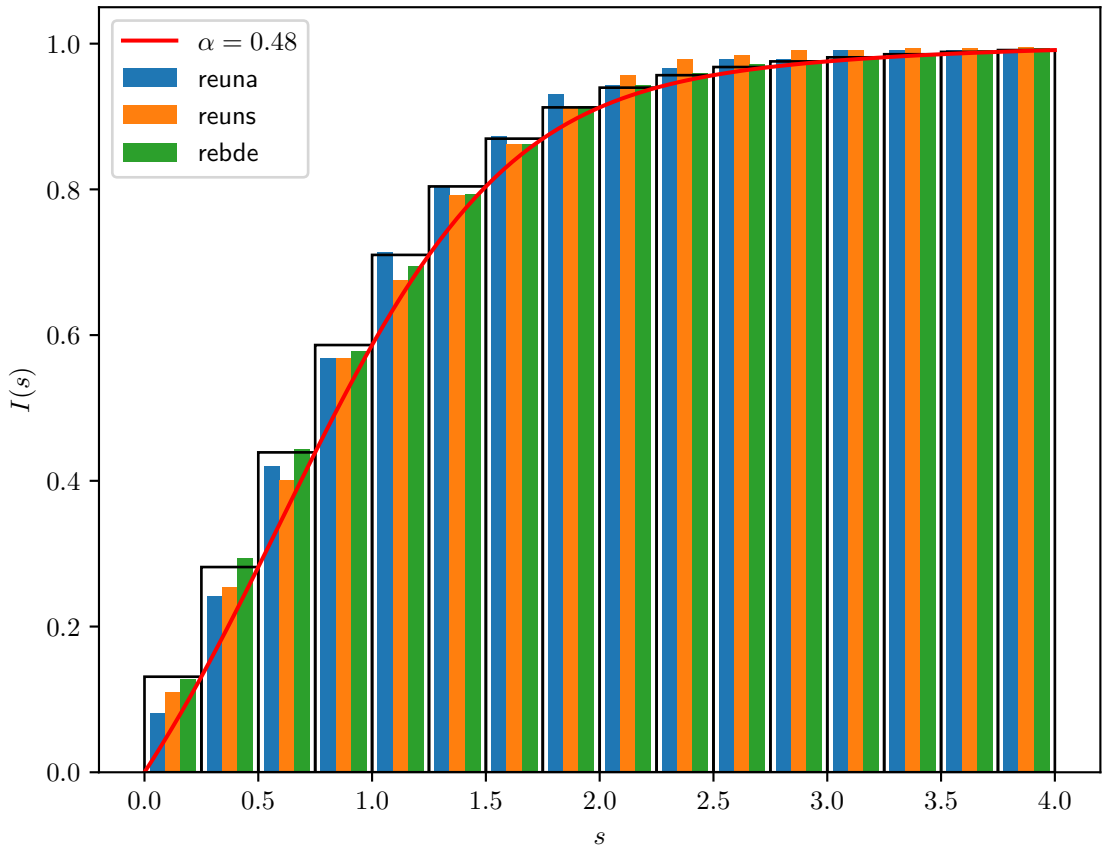


Figure 5.4: $B = 0.63, D = 0.4, N = 260$

Chapter 6

Conclusions