Chapter 1

Procedure

1.1 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 two dimensional oscillator has a *zero point motion* with the energy equal to $\hbar\omega_0$. Since we are interested in the spacings between consecutive, we can rescale the 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 $a_1^{\dagger n_1} a_2^{\dagger n_2}$ we generate 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

$$\begin{aligned}
H = A\left(a_1^\dagger a_1 + a_2^\dagger a_2\right) + \frac{B}{4}\Big[& \left(3a_1^\dagger {a_2^\dagger}^2 + 3a_1 a_2^2 - {a_1^\dagger}^3 - a_1^3\right) \\
& + 3\left(a_1 {a_2^\dagger}^2 + a_1^\dagger a_2^2 - a_1^\dagger a_1^2 - {a_1^\dagger}^2 a_1 + 2a_1 a_2^\dagger a_2 + 2a_1^\dagger a_2^\dagger a_2\right)\Big] \\
& + \frac{D}{16}\Big[6\left({a_1^\dagger}^2 a_1^2 + {a_2^\dagger}^2 a_2^2\right) + 2\left(a_1^2 {a_2^\dagger}^2 + {a_1^\dagger}^2 a_2^2\right) + 8a_1^\dagger a_1 a_2^\dagger a_2 \\
& + 4\left(a_1^\dagger a_1^3 + {a_1^\dagger}^3 a_1 + a_2^\dagger a_2^3 + {a_2^\dagger}^3 a_2 + a_1^2 a_2^\dagger a_2 + {a_1^\dagger}^2 a_2^\dagger a_2 + a_1^\dagger a_1 a_2^2 + a_1^\dagger a_1 {a_2^\dagger}^2\right) \\
& + \left({a_1^\dagger}^4 + a_1^4 + {a_2^\dagger}^4 + a_2^4 + 2{a_1^\dagger}^2 {a_2^\dagger}^2 + 2a_1^2 a_2^2\right)\Big].
\end{aligned} \tag{1.1}$$

The physical origin of this Hamiltonian is related to quadrupole dynamics of nuclear surfaces[1, 2]. The operators a_1 and a_2 are related to the normal modes of the quadrupole vibrations. In the case of a deformed nucleus, one mode named β-vibration corresponds to oscillations preserving the axial symmetry. For the second mode, γ-vibrations, the transversal section perpendicularly to the symmetry axis changes periodically from ellipse to circle.

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 diagonalisation routine based on Relatively Robust Representations from Intel® Math Kernel Library [3] used via a `Python` program [4, 5, 6]Any such diagonalisation 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 diagonalisation basis as is detailed in the next section.

1.2 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 $N = 140$.

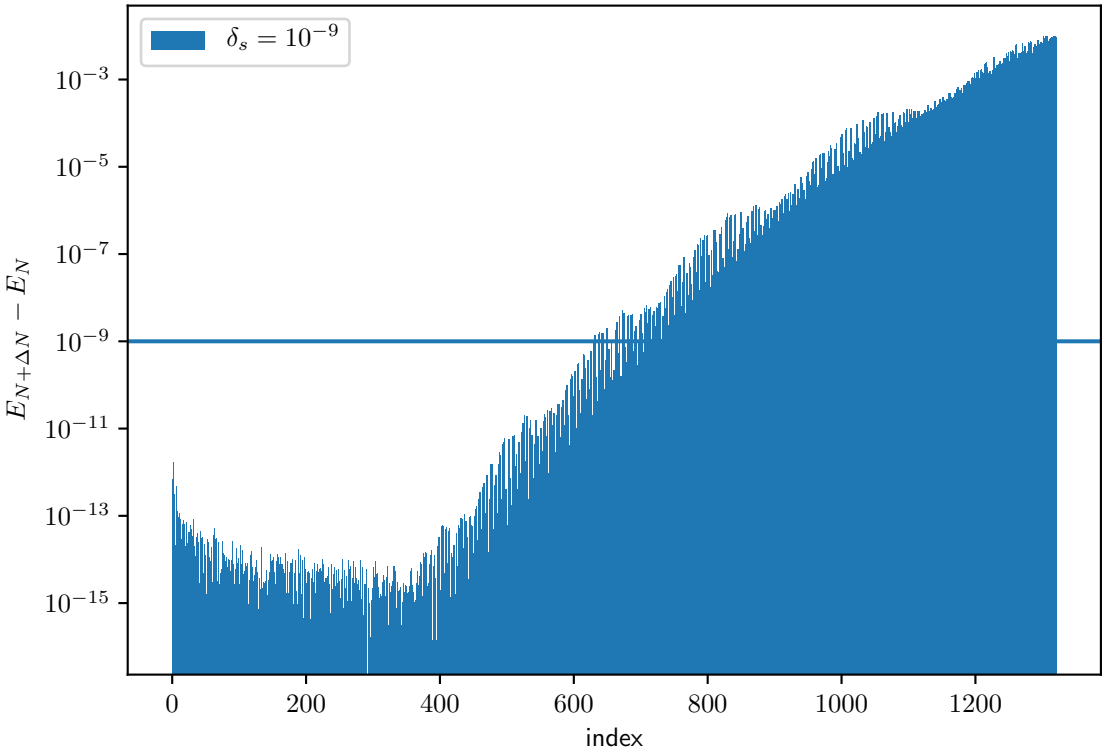


Figure 1.1: $B = 0.2, D = 0.4, N = 120$

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 $N = 280$

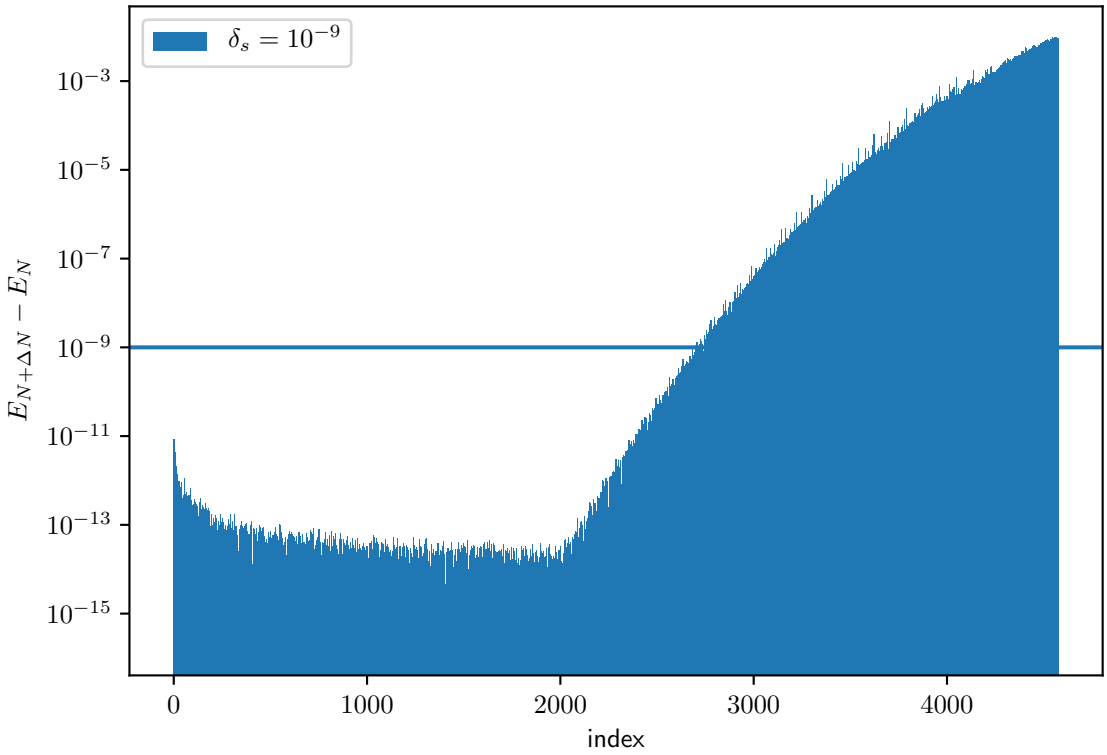


Figure 1.2: $B = 0.55, D = 0.4, N = 260$

As expected, the number of stable levels increases with the diagonalisation 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 $\Delta N = 20$.

1.3 Statistics

As mentioned in **??**, 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 diagonalisation. 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*,

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

1.3.1 Irreducible representations

In order to analyse the distributions of the previously obtained eigenvalues we must first take into account the possible symmetries of the system. A consistent analysis requires us to consider classes of states which transform with the same *irreducible representation*.

The Hamiltonian in eq. (1.1) has the finite $\mathcal{C}_{3v}$ symmetry group. This group has 3 irreducible representations: one bi-dimensional and two unidimensional, one symmetric and one anti-symmetric, namely $\Gamma_b, \Gamma_s, \Gamma_a$.

Separating the bi-dimensional representation

The presence of the bi-dimensional representation corresponds a two-fold degeneracy. These degeneracies can be identified by scrutinising the differences between consecutive levels $\Delta E = E_{i+1} - E_i$. An other option is to use directly the relative spacing, which is a rescaling in units of average separation. The separation of the symmetric and anti-symmetric irreducible representations will be detailed later.

In figure 1.3 we can see how ΔE varies with the index of the levels.

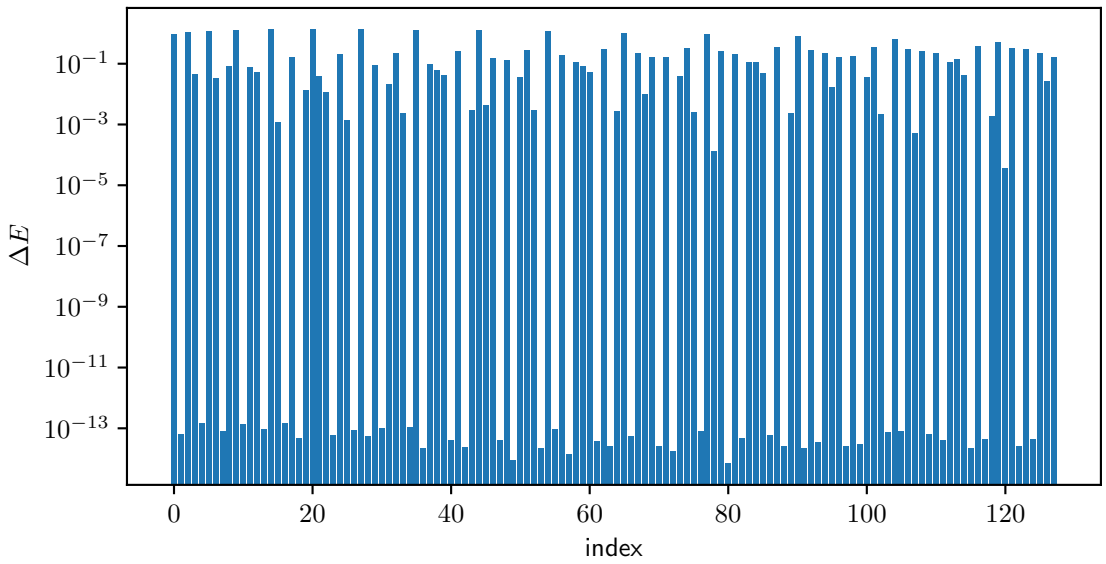
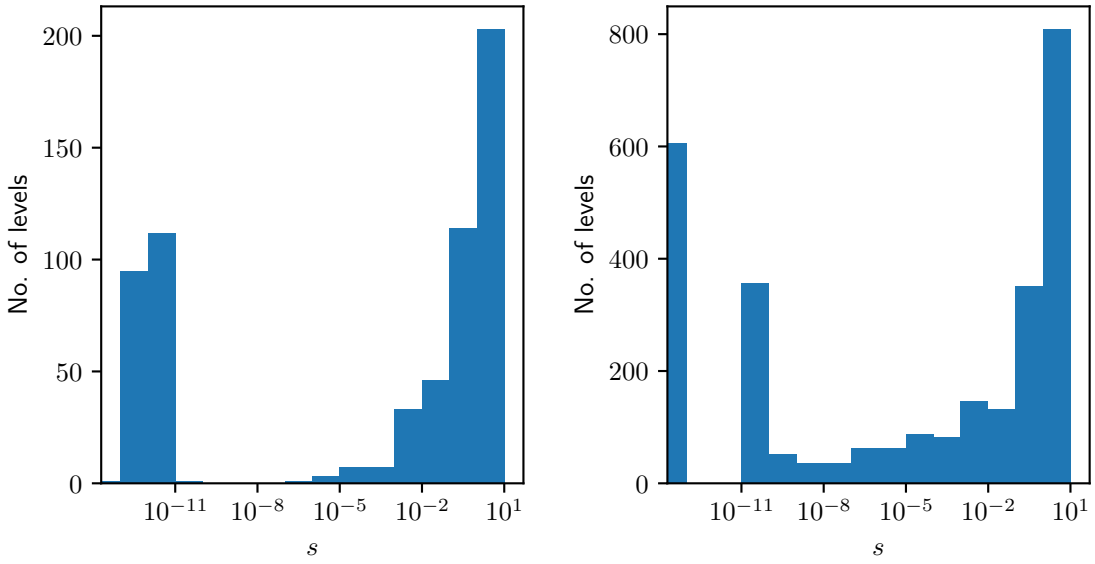


Figure 1.3: $B = 0.2, D = 0.4, N = 60$

Due to 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 as belonging 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 1.4a).

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



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

Figure 1.4: The relative spacing histograms for different parameters

$B = 0.4$) 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 very low values. (see fig. 1.4b)

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 a clear separation of the spacings corresponding to the bi-dimensional representation (see fig. 1.5).

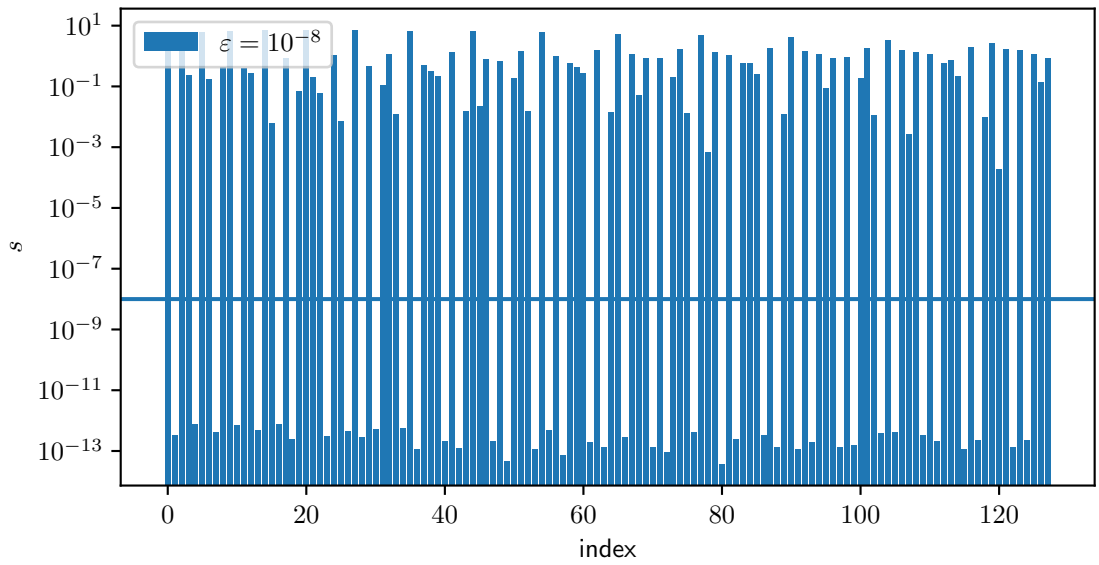


Figure 1.5: $B = 0.2, D = 0.4, N = 60$

Separating the unidimensional representations

The unidimensional representations can be distinguished from the properties of the states at reflections with respect to the Ox axis ($y \rightleftarrows -y$). We ca establish a correspondence between the symmetry of the states to this operation and the values of the quantum number n_2. The states containing dominantly oscillator ket vectors with even n_2 will transform with the symmetric representation.

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

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

In figures 1.6 and 1.7, respectively 1.8 and 1.9 we can see the relative spacing for each irreducible representation as a function of index and as a histogram for $B = 0.2$ and $B = 0.63$. Once the problem of selection of the states corresponding to a given irreducible representation was solved, we calculated the average spacing for different values of B (see fig. 1.10).

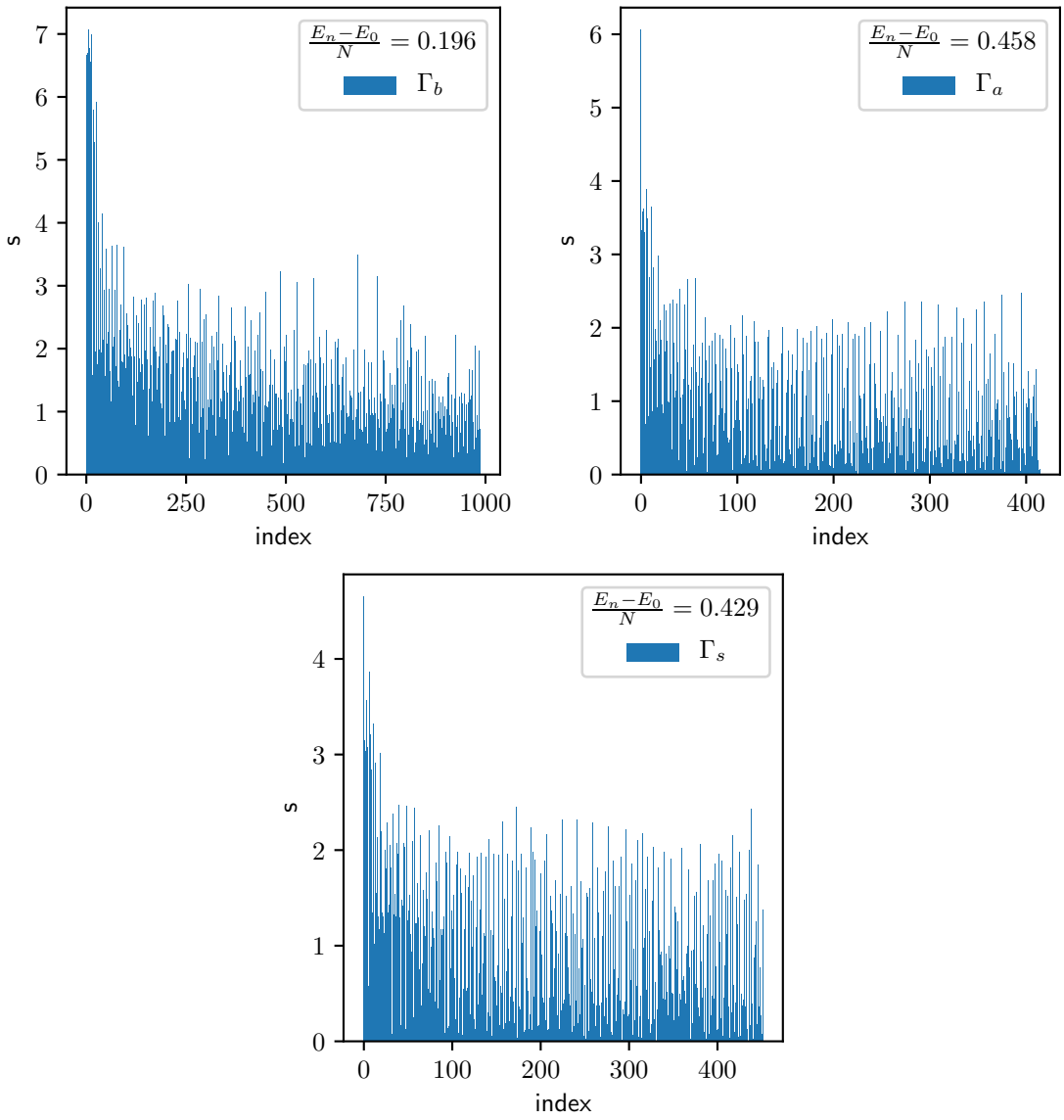


Figure 1.6: The relative spacing for each irreducible representation as a function of index for $B = 0.2, D = 0.4, N = 260$

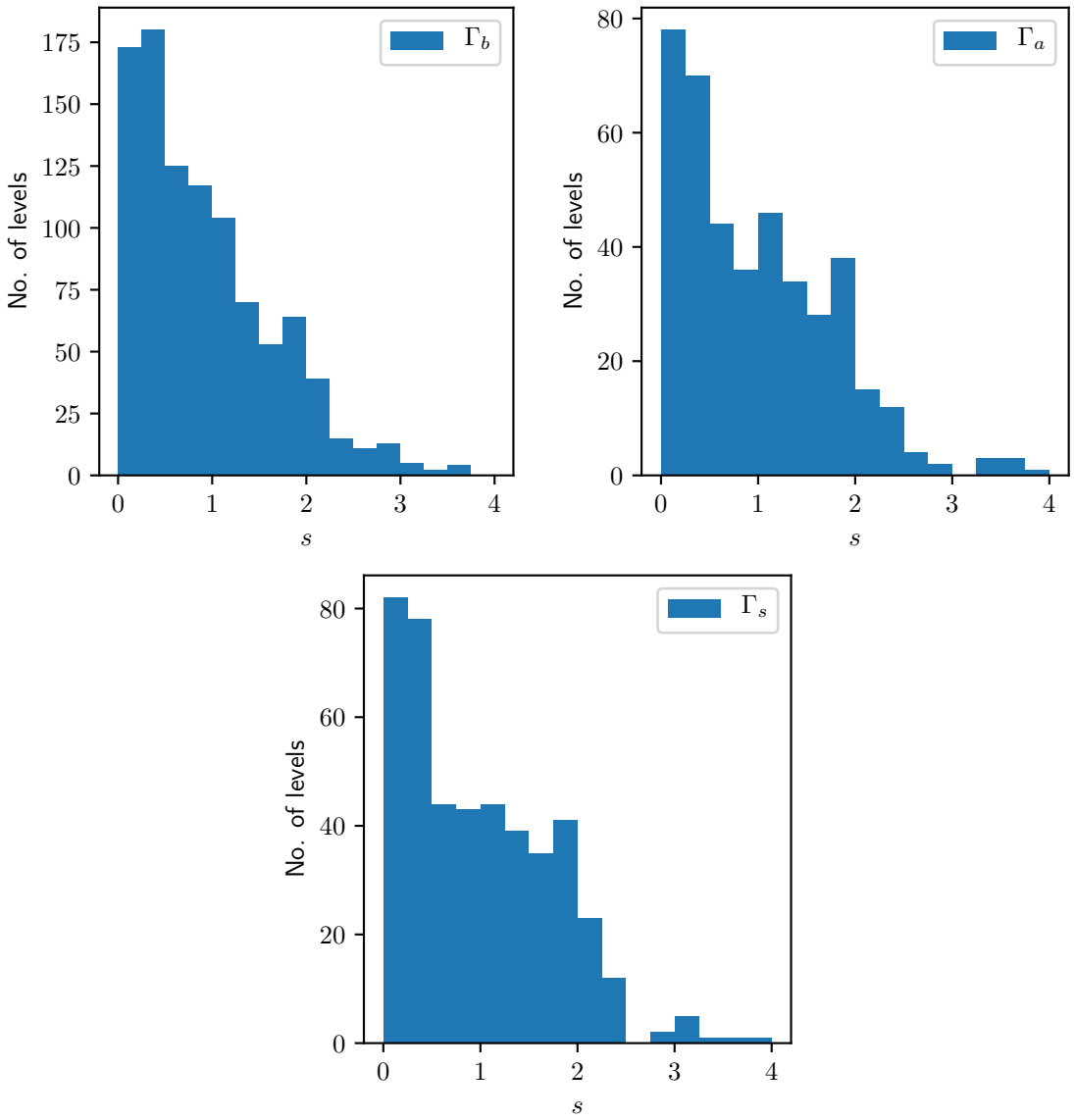


Figure 1.7: The relative spacing histogram for each irreducible representation for $B = 0.2, D = 0.4, N = 260$

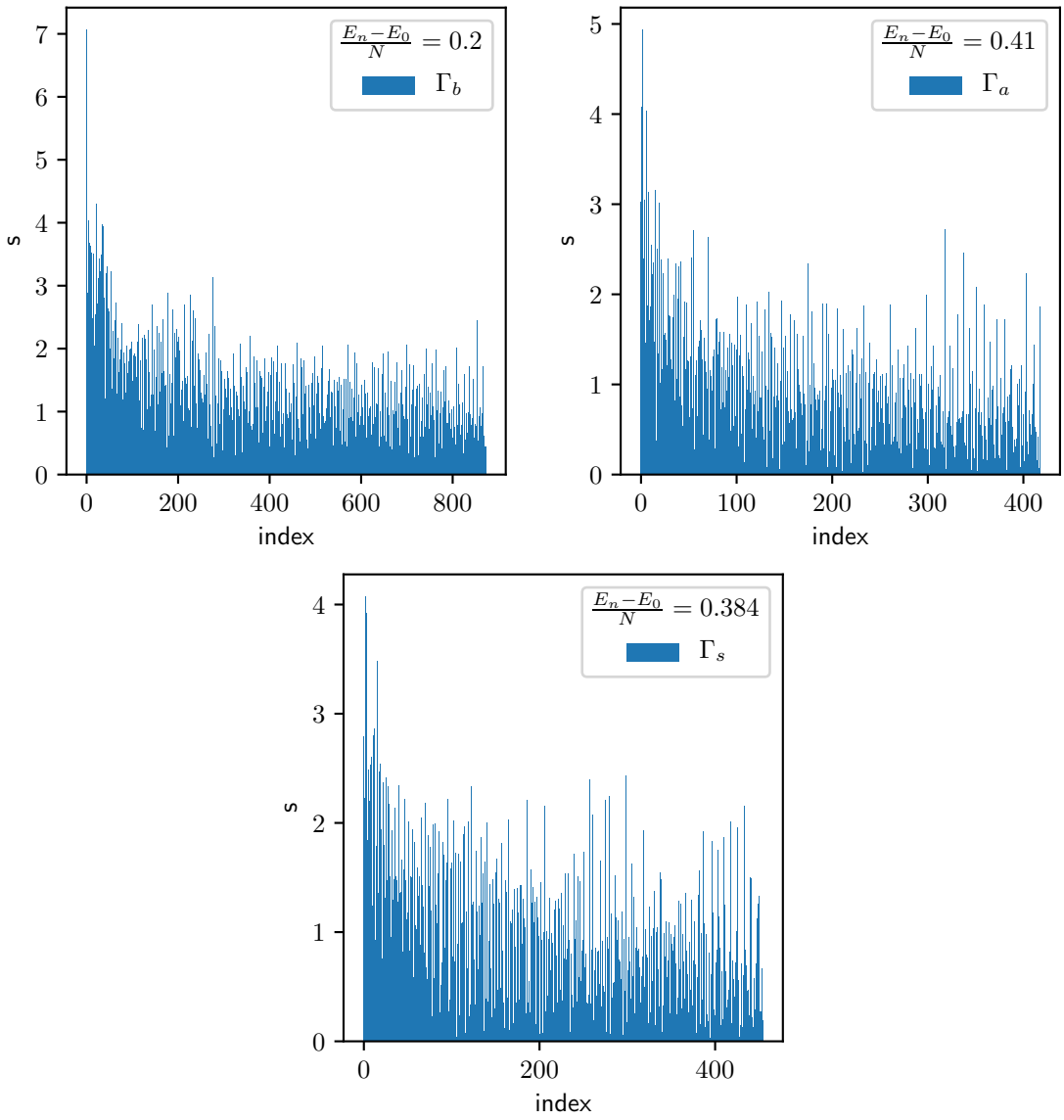


Figure 1.8: The relative spacing for each irreducible representation as a function of index for $B = 0.63, D = 0.4, N = 260$

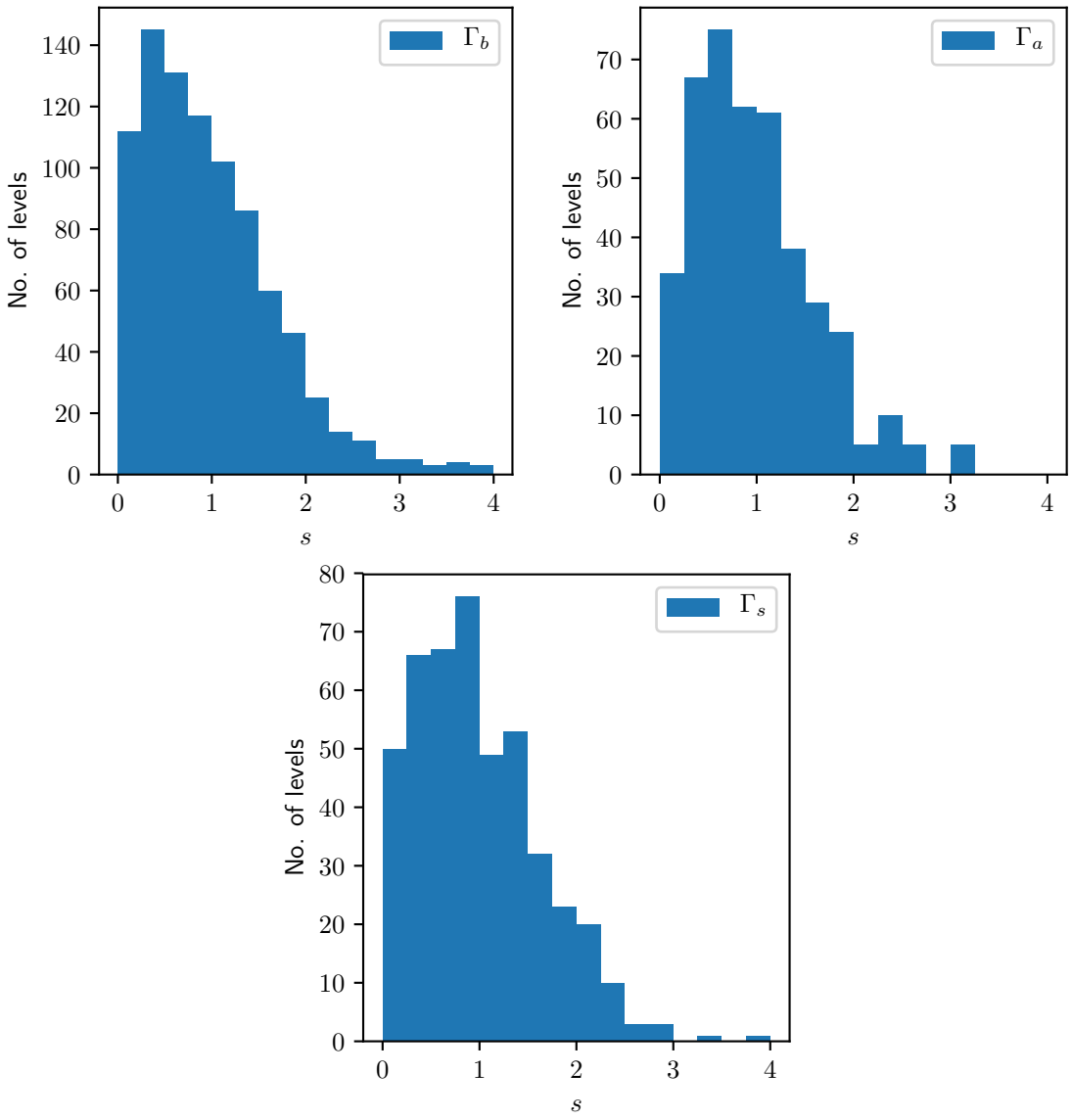


Figure 1.9: The relative spacing histogram for each irreducible representation for $B = 0.63, D = 0.4, N = 260$

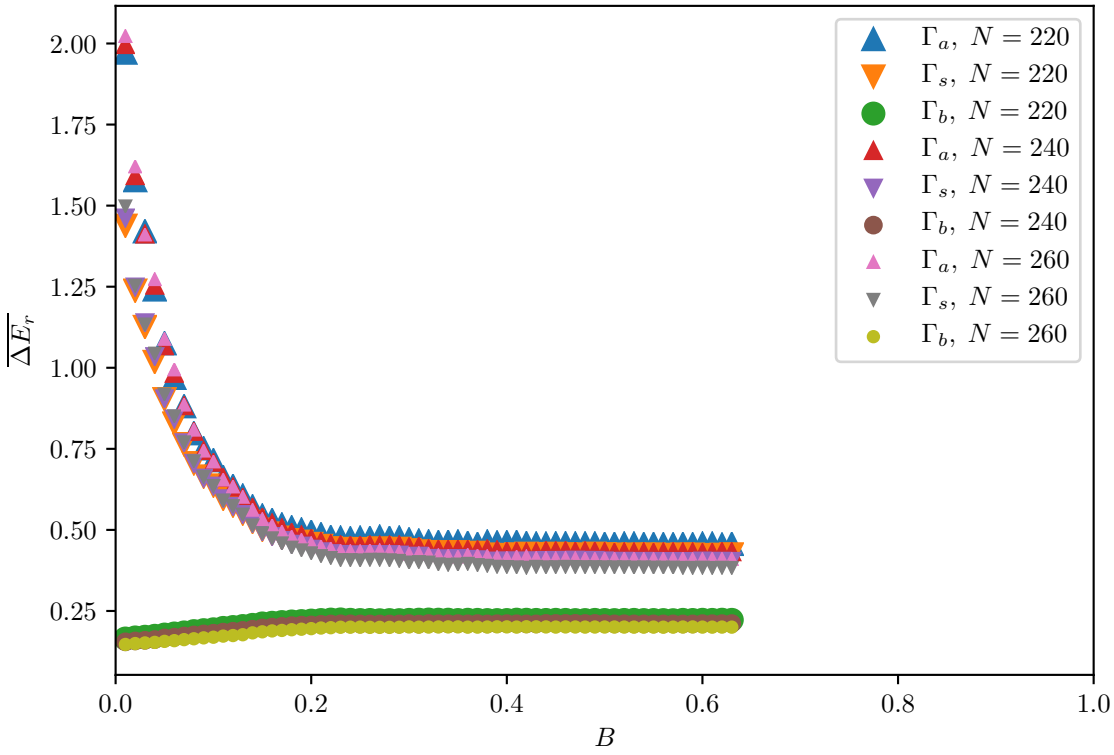


Figure 1.10: $\overline{\Delta E}$ as a function of B for each representation

1.3.2 Nearest neighbour distributions

Having separated the states with respect irreducible representations we can also build the nearest neighbour distributions. These histograms show the probability of having a given spacing between consecutive levels as a function of s.

Figures 1.11 to 1.14 show the nearest spacing distributions $P(s)$ and the cumulative distributions $I(s)$ for $B = 0.2$ and $B = 0.63$.

Taking into account the Berry-Tabor and Bohigas-Gianoni-Schmit conjectures, we compare $P(s)$ with the Poisson distribution $P_P(s) = \mathrm{e}^{-s}$ and the Wigner distribution $P_W(s) = \frac{\pi}{2} s \exp\left(-\frac{\pi}{4} s^2\right)$.

Since $P(s)$ is a histogram, for an easier comparisom, we also computed the histograms associated with the two distributions for the same spacing.

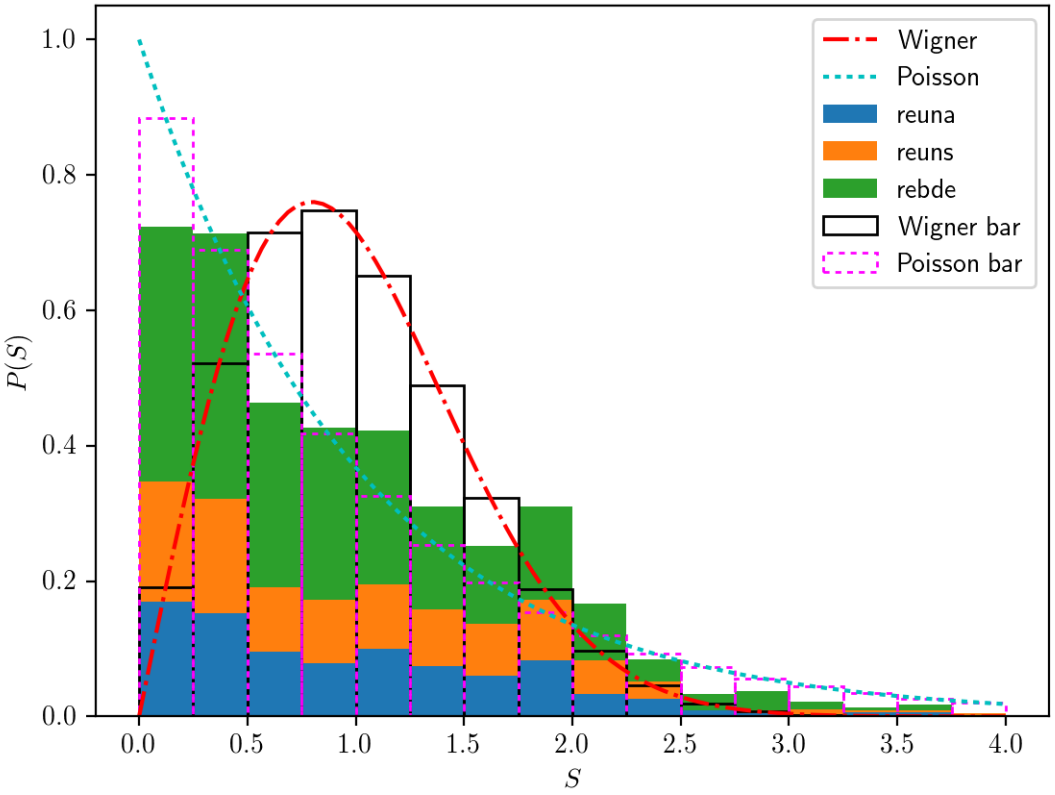


Figure 1.11: $B = 0.2, D = 0.4, N = 120$

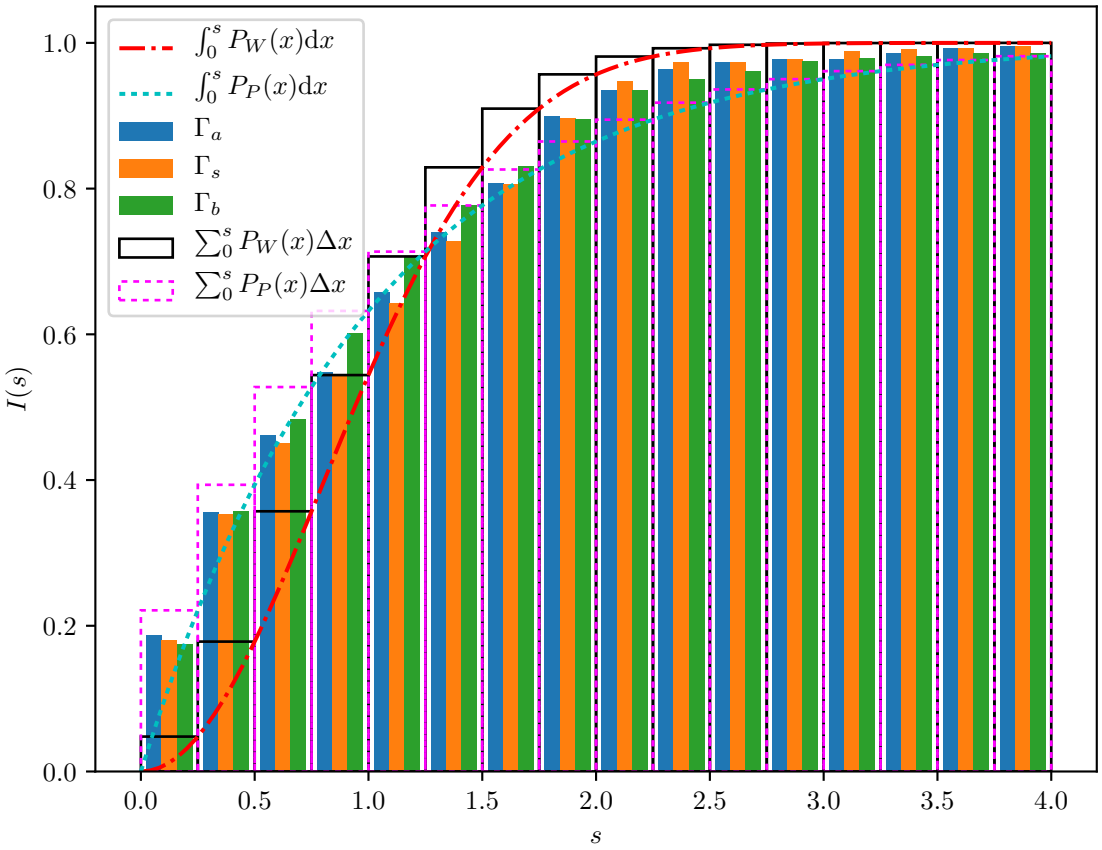


Figure 1.12: $B = 0.2, D = 0.4, N = 120$

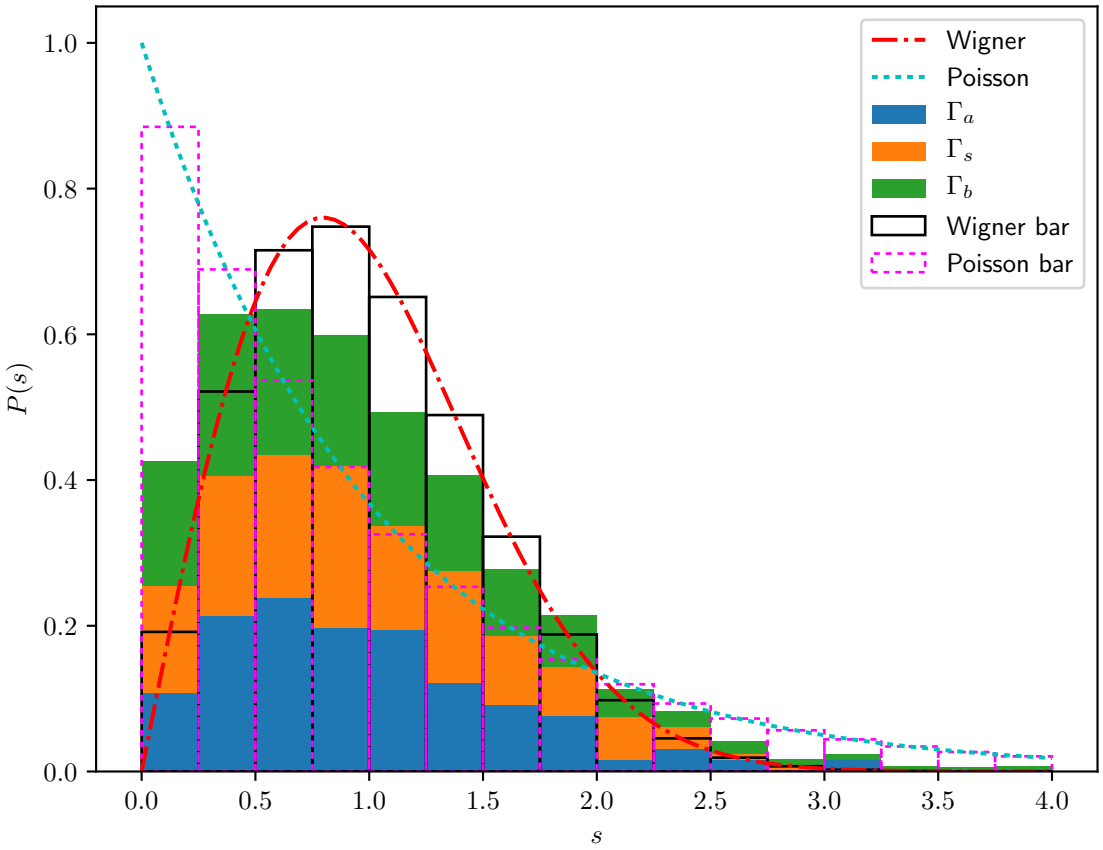


Figure 1.13: $B = 0.63, D = 0.4, N = 260$

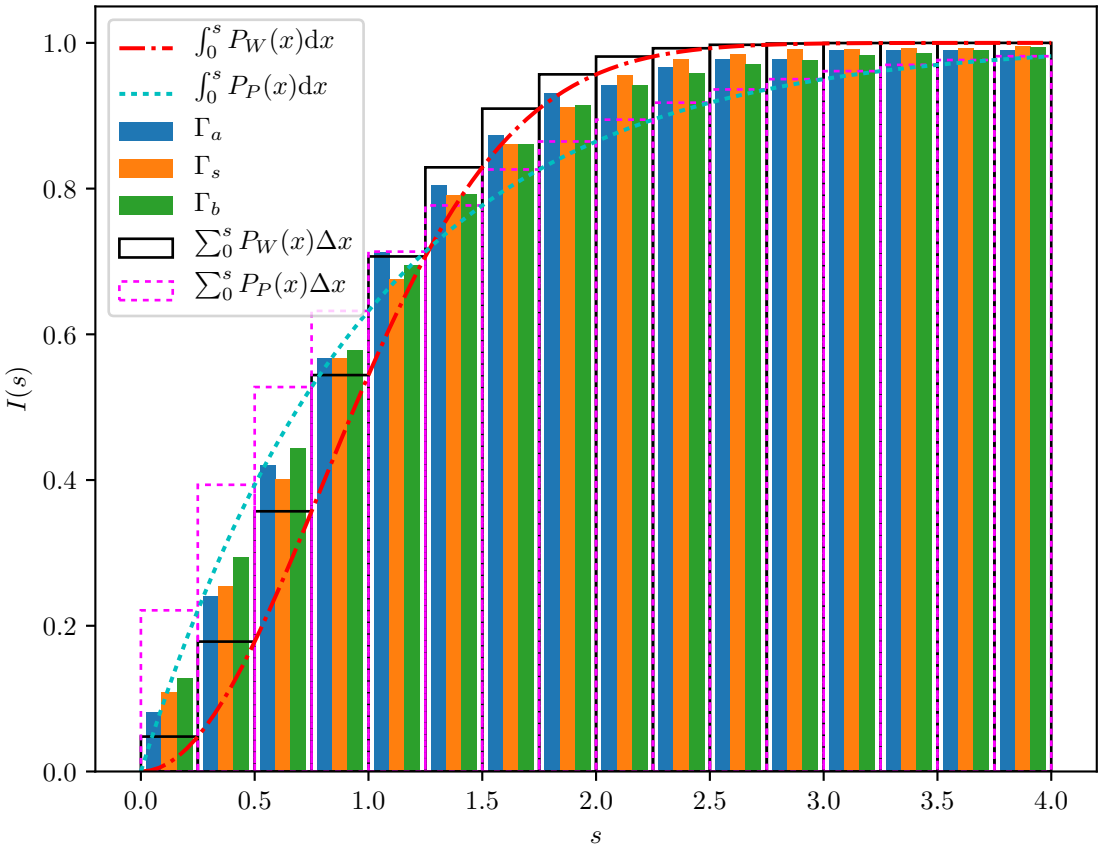


Figure 1.14: $B = 0.63, D = 0.4, N = 260$