

**DEVELOPMENT OF A NOVEL ALGORITHM FOR NUCLEAR
LEVEL SCHEME DETERMINATION**

A Thesis

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GREGORY A. DEMAND

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ABSTRACT

DEVELOPMENT OF A NOVEL ALGORITHM FOR NUCLEAR LEVEL SCHEME DETERMINATION

Gregory A. Demand
University of Guelph, 2009

Advisor:
Professor Paul Garrett

Modern γ -ray spectrometers are capable of performing experiments involving the collection of high-statistics data sets containing information on hundreds of transitions. The information extracted from the data sets are usually presented in the form of level schemes. However, the process of constructing nuclear level schemes can take months to years, greatly inhibiting the progress of nuclear physics - especially when investigating trends amongst nuclei. In this thesis an analytical formula that directly relates nuclear level schemes to experimental data, and a transition-centric level scheme representation are developed. The analytical formula was successfully tested on simulated directed data including irresolvable doublets, and a self-consistent approach to undirected data was investigated. Furthermore, a variety of computer automated methods involving the analytical formula, the transition centric representation, and evolutionary computation are investigated. Simulated doublet-free level schemes with up to 150 transitions and 60 levels were determined using these methods.

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Chapter 1

Introduction

1.1 Motivation

A significant portion of nuclear physics requires knowledge of nuclear level schemes. Nuclear level schemes are frequently constructed from γ -ray spectroscopy experiments. The continuing development of modern spectrometers, which have high efficiencies and which may be sensitive to high multiplicity events, can lead to measurements with very high statistics. The resulting data sets are often extremely complex, and can contain more than 200 transitions. As a result, determining and verifying the accuracy of level schemes is generally a very time consuming process. This time requirement is a substantial obstacle to the progress of nuclear physics - especially due to the need for nuclear structure investigations to examine trends across many nuclei.

There is significant variety in the data sets produced by different γ -ray spectroscopy experiments. One way in which these experiments vary is in the mechanism used to excite the nuclei. Using different excitation mechanisms changes what aspects of the nuclei of interest the experiment is sensitive to. One class of excitation mechanisms consists of low-spin processes such as β decay. A characteristic of this

class of excitation mechanisms is that nuclei are excited to many levels with the same spin. This results in very dense level schemes, with transitions observed in most allowed locations, such as the level scheme presented in Figure 1.1. This is in contrast with high-spin reactions such as fusion evaporation reactions that typically observe transitions close to the yrast band over a large spin range. This results in a relatively sparse level scheme, containing long chains of transitions with predictable energies, as in Figure 1.2, though the low-spin regions of these experiments are often dense. Due to these characteristics, low-spin experiments, and the low-spin regions of high-spin experiments tend to produce very complicated data sets that are an excellent target for computer automation.

Increases in computational power, while insufficient for determining level schemes by brute-force, make possible the development of algorithmic approaches to level scheme determination. The development of efficient and accurate algorithms would greatly decrease the time required to analyze complicated nuclear physics experiments, thereby facilitating nuclear physics research, especially in the case of low-spin nuclear spectroscopy.

1.2 Outline

This thesis consists of a chapter of background material, followed by a discussion of various approaches to automated nuclear level scheme determination. Background material for both the nuclear physics and the mathematical aspects of the thesis is presented in chapter two. Chapter three develops and discusses an analytical formula for calculating level schemes from directed experimental data. In chapter four the results of using the analytical formula developed in chapter three and a related self-consistent equation for determining level schemes from simulated data are presented. Chapter five demonstrates three different approaches to determining nuclear level

schemes using evolutionary algorithms. Conclusions and possible directions for future work are found in chapter six. Appendix A contains level space schemes represented in transition space. Appendix B discusses converting level schemes from transition space to level space.

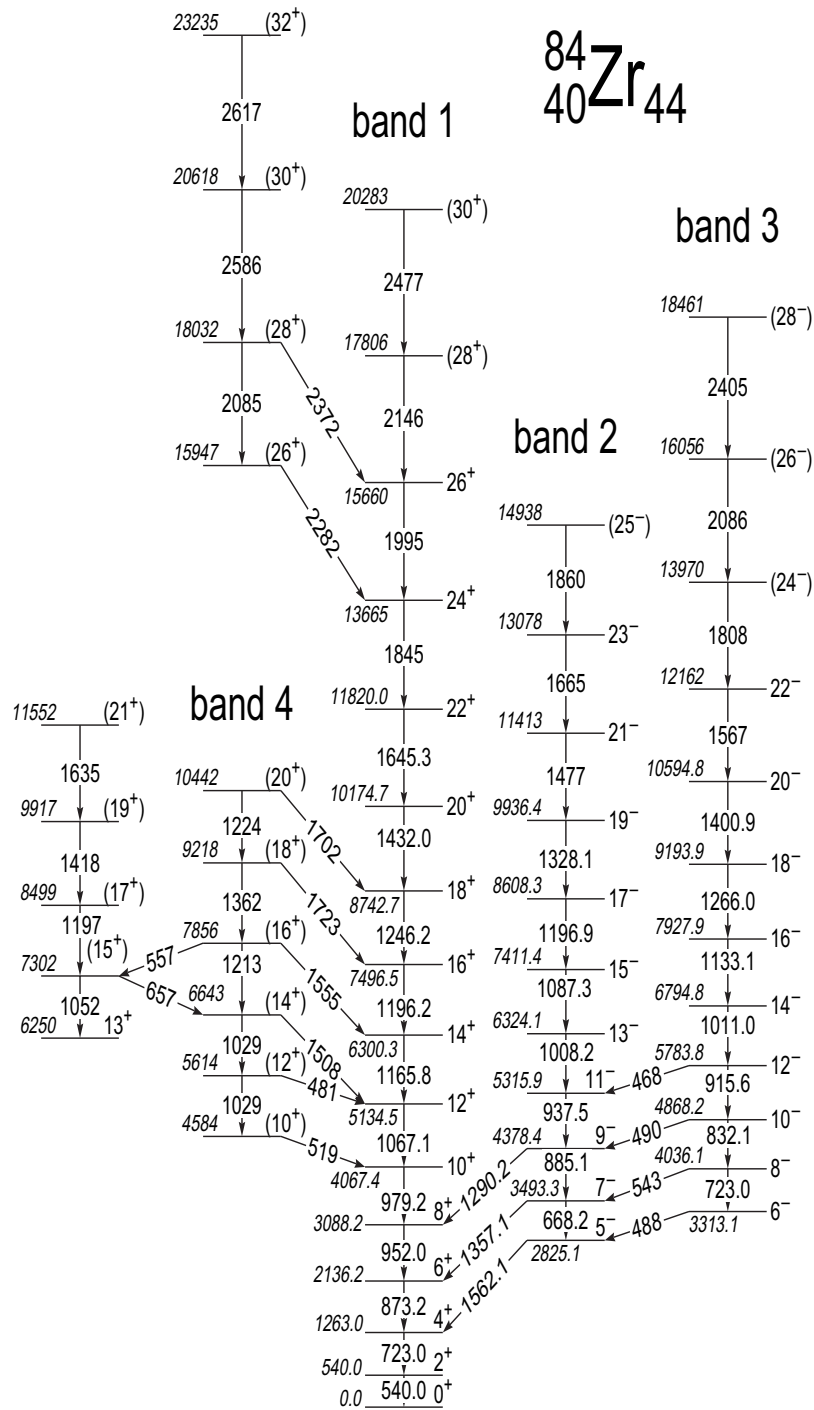


Figure 1.2: A partial ^{84}Zr level scheme produced from a high-spin fusion-evaporation reaction. In this scheme there are several long rotational bands, with few cross transitions between the bands [2].

Chapter 2

Background

2.1 Experimental Background

2.1.1 Experimental Data Collection

Nuclear spectroscopy experiments are often performed using large arrays of γ -ray detectors such as the 8π [3] at TRIUMF-ISAC [4] illustrated in Figure 2.1. The 8π consists of multiple detector systems, including an array of 20 high-purity germanium detectors. These germanium detectors detect the γ rays produced when a nucleus decays from one energy level to another, and the measured γ rays are associated with transitions in the level scheme. Since the typical characteristic half-lives of nuclear energy levels are less than the detector time resolution (nanoseconds), γ rays that are detected at the same time (in coincidence) in different detectors will be associated with the same decay path in the level scheme. (Taking into account effects such as background radiation, random coincidences and detector behaviour.) A 2-dimensional histogram called a coincidence matrix which gives the number of times γ rays with each pair of energies were detected is created. A singles spectrum - a 1-dimensional histogram giving the number of times a γ ray with each energy was detected - is also constructed.

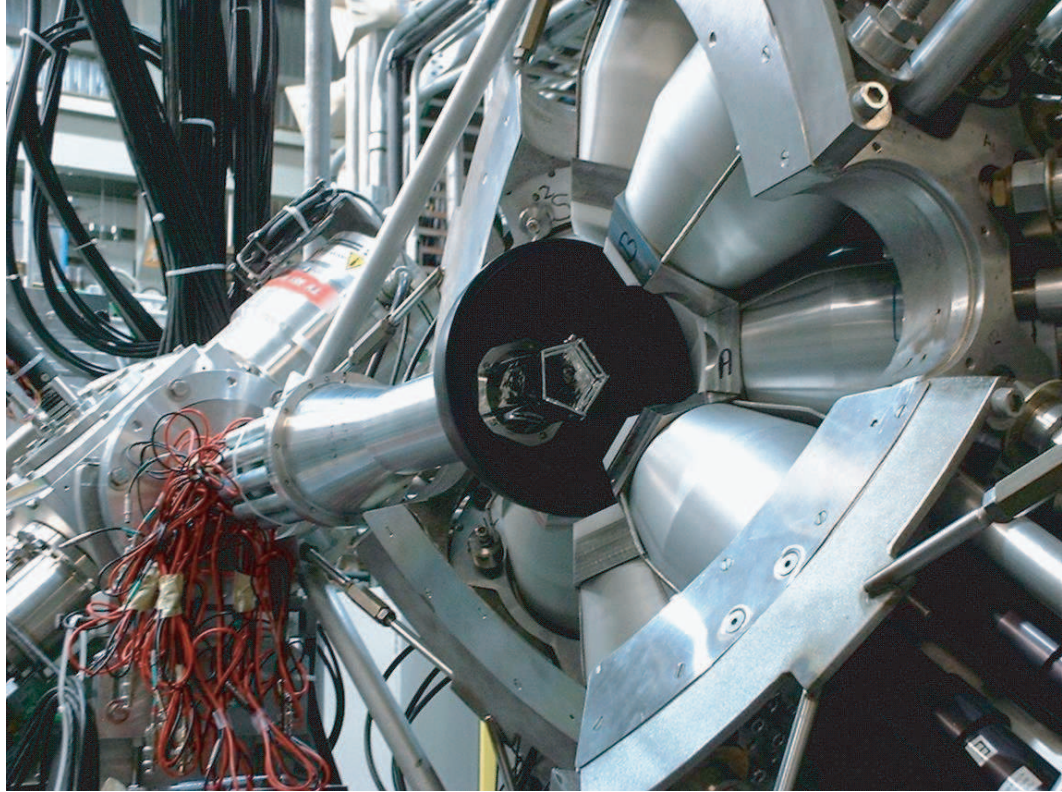


Figure 2.1: The 8π located at TRIUMF-ISAC is a large high efficiency γ -ray spectrometer consisting of 20 high purity germanium detectors which are complemented by the SCEPTAR, DANTE and PACES auxiliary detection systems.

2.1.2 Level Scheme Construction

Currently, nuclear level schemes are constructed from γ -ray spectroscopy data by iteratively looking for patterns in the coincidence matrix, adding transitions to a trial level scheme, then checking if the new trial level scheme corresponds with the coincidence matrix [5]. This process can be quite time consuming (many months to years) as many level schemes are complex and involve large numbers of transitions. As a result, the determination of level schemes can become a substantial obstacle to the rapid development and formulation of new ideas.

2.2 Mathematical Background

2.2.1 Graph Theory

Graphs are an excellent mathematical tool for representing networks [6]. In general a graph consists of a set of vertices V and a set of edges E . Vertices represent states, and edges represent connections between states. A graph can be either directed or undirected. In directed graphs, edges represent one-way connections. Examples are found in Figure 2.2.

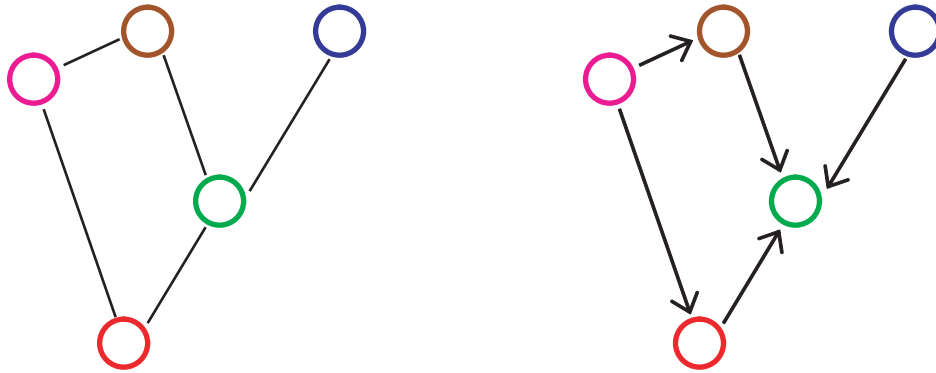


Figure 2.2: An undirected and a directed graph.

Edges in graphs can be weighted. The weighting of an edge can have many meanings - it can represent the number of paths, the distance between vertices or the probability of traversing the edge. Graphs containing weighted edges are referred to as weighted graphs, such as the graph in Figure 2.3.

Level schemes can be represented as weighted directed graphs. In this representation, levels are represented as vertices and transitions are represented as edges. The weighting of an edge gives the branching ratio (or probability of traversal) for the associated transition. Level energies are represented as the height of the vertex in the scheme. The other characteristics of the energy levels and transitions are associated with the appropriate vertices and edges, but they are not a fundamental part of the graph.

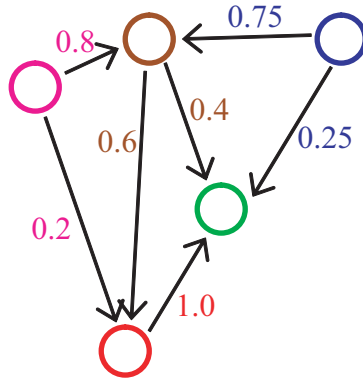


Figure 2.3: A weighted directed graph where the weights represent the probability of traversing the edges.

Adjacency matrices are a common representation of graphs. For a level scheme, the adjacency matrix A is a matrix where element $A_{i,j}$ gives the probability of i decaying to j , as shown in Figure 2.4. The adjacency matrix can be formed by taking the branching ratios of a level scheme and placing them in the appropriate locations. An adjacency matrix contains all information required to build a level scheme.

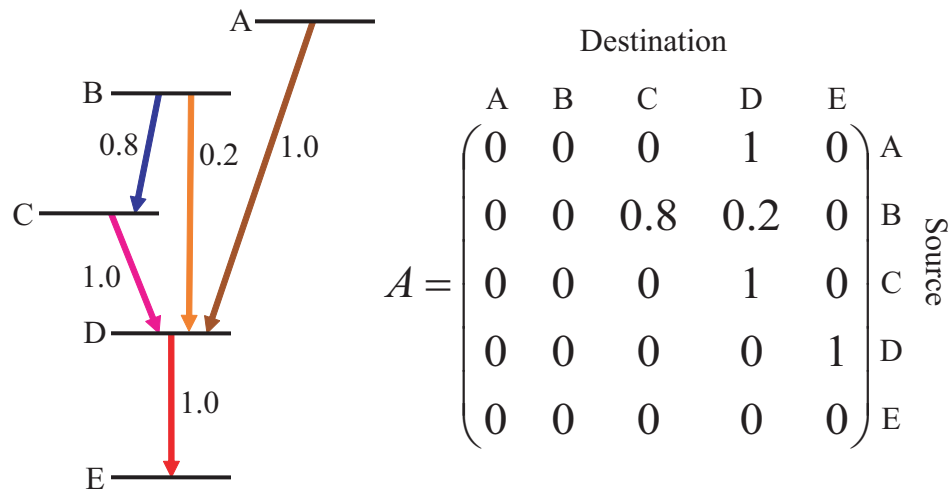


Figure 2.4: A level scheme and the associated adjacency matrix.

2.2.1.1 Line Graphs

Line graphs are a method of representing the adjacencies between the edges of a graph. The line graph of an undirected graph is an undirected graph with one vertex for every edge in the original graph, where edges between vertices indicate that the associated edges are adjacent in the original graph. Line graphs of directed graphs can be constructed in the same way, except that the resultant line graph will be directed, and that an edge from vertex A to vertex B in the line graph indicates that the destination of the edge associated with A is the source of the edge associated with B . A directed graph and associated line graph are presented in Figure 2.5.

The line graph of a level scheme is a graph where vertices represent transitions, and edges indicate that the first transition decays to the second transition in one step. As discussed in Section 2.2.2.2, this indicates that there are no observed transitions between the two transitions, and as a result the destination energy level of the first transition is probably the source energy level of the second transition. Line graphs of level schemes contain decay path information in a transition centric form, and will be used as the basis for transition space level schemes.

2.2.1.2 Total Probability Formula

For weighted graphs, where edge weighting represents the branching ratio, it is possible to mathematically relate the probability of decaying between two vertices to the adjacency matrix.

The element $A_{i,j}$ of the adjacency matrix gives the probability of directly decaying from vertex i to vertex j . Using matrix multiplication it follows that $A_{i,j}^2$ gives the probability of directly decaying from vertex i to vertex j in two steps. This argument can be extended through induction to prove that the probability of decaying from i to j in n steps is given by A^n .

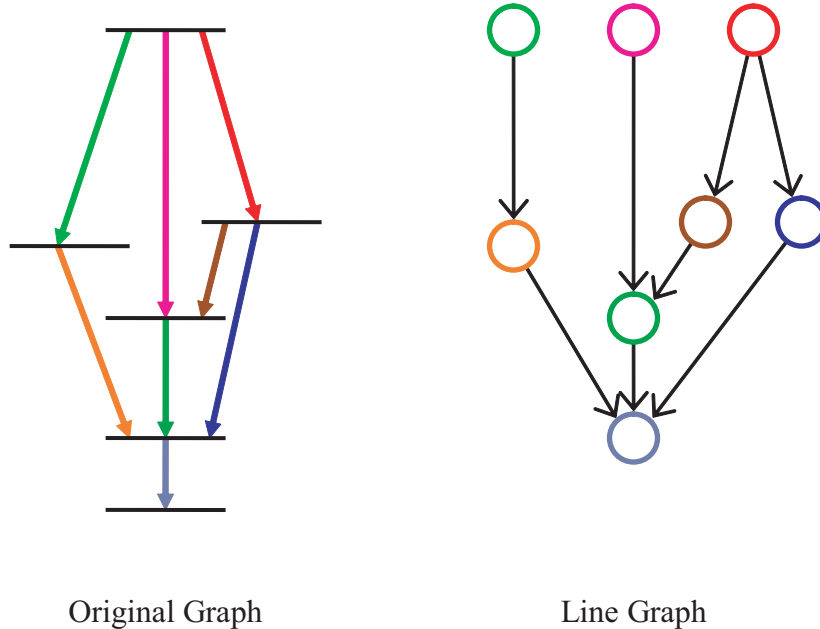


Figure 2.5: A directed graph and associated line graph.

From this it follows that P , the total probability of decaying from i to j is:

$$P = A + A^2 + A^3 + \dots \tag{2.1}$$

The identity:

$$I + A + A^2 + \dots = (I - A)^{-1} \tag{2.2}$$

can be rearranged to match the form of Equation (2.1):

$$A + A^2 + A^3 + \dots = (I - A)^{-1} - I. \tag{2.3}$$

Thereby allowing us to replace the infinite sum with a matrix inversion, giving

$$P = (I - A)^{-1} - I. \tag{2.4}$$

This formula will be used in Section 3.3.

2.2.2 Transition Space

Nuclear spectroscopy experiments extract information by examining the γ rays emitted from nuclei. These γ rays encode information about transitions and the relationships between them. As a result, it is logical to analyze these experiments using a transition-centric representation, as in Figure 2.6.

Level schemes are traditionally denoted in a very level-centric fashion, with levels represented as vertices and transitions represented as edges. If one transition feeds into another transition, it is denoted as a transition feeding into a level that happens to decay into the second transition - even though the experimental data contains no information about the intermediate level. This representation will be referred to as level space.

In transition space, transitions are represented as vertices. The abstract connections between transitions are represented as edges. The simplest edges represent that the transitions are connected through a single level. However, they can also represent a sequence of levels with unobserved γ rays connecting the levels, as per Figure 2.7. Additionally, there is not a one-to-one correspondence between edges and levels, as each level is capable of connecting more than one pair of transitions.

Since the vertices in transition space are associated with transitions, the adjacency matrix can be used to directly model the relationships between transitions, as in Figure 2.8. This allows us to create equations relating experimental data directly to level scheme structure.

As an important note, energy is still represented as the height of a vertex. However, since vertices now represent transitions, the height of a vertex now represents either the starting energy or the destination energy of a transition, rather than the energy of a level. In the present work height will be used to represent starting ener-

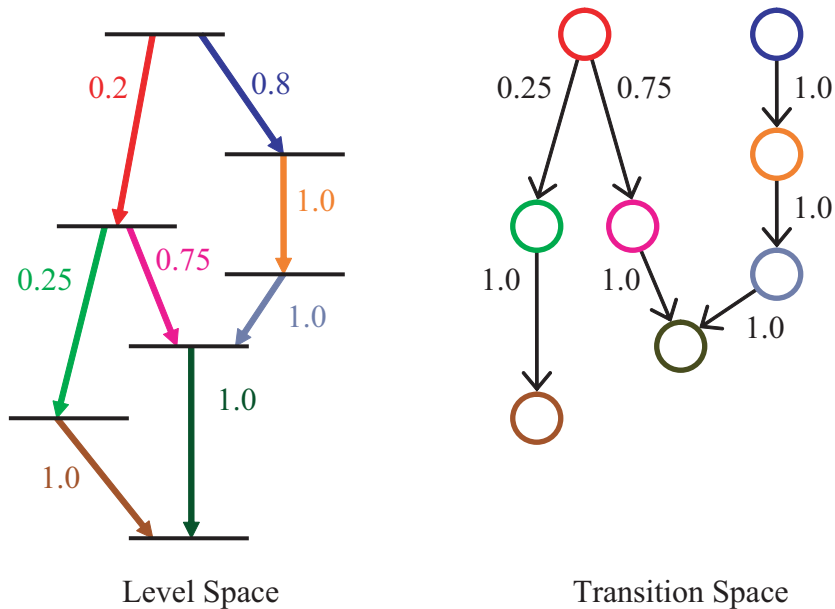


Figure 2.6: A level space scheme and the associated transition space scheme. The branching ratios in the transition scheme are equal to the probability of decaying through the destination transition given that the nucleus decayed through the source transition. As a result, since there is no transition decaying into the top level of the level space scheme, the branching ratios from the top level are not present in the transition space scheme. As a note, these branching ratios cannot be directly observed in a γ -ray spectroscopy experiment, though they would be implicitly included in the singles data.

gies of transitions. One difficulty with representing the starting energy of transitions as height in transition space is that the energies of unobserved transitions must be accounted for. For example, looking at Figure 2.9, if two transitions are connected by an edge that represents two levels connected by a 120 keV transition, the starting energy of the initial transition will be off by 120 keV if it is naively assumed that the edge represents a single level.

While the possibility of unobserved transitions makes it more difficult to accurately determine the starting energies of the transitions, it gives us a tool for locating unobserved transitions in the level scheme. If the calculated starting energy of a transition differs by 30 keV depending on which decay path is followed, it implies

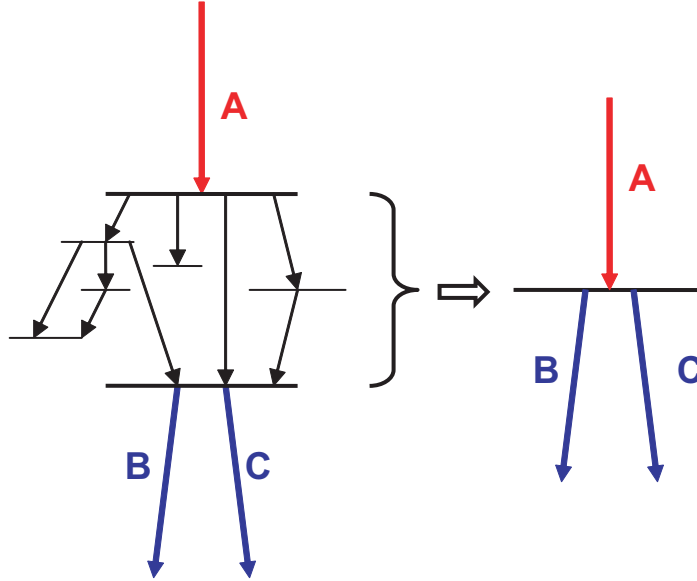


Figure 2.7: Both of these level space schemes would be represented as a pair of edges (one connecting A to B, and one connecting A to C) in transition space, since the experimental data contains no information about the unobserved transitions.

that there is an unobserved transition of 30 keV along the ‘shorter’ decay path, as in Figure 2.10.

2.2.2.1 Switching Between Transition Space and Level Space

A level space scheme can be converted to a transition space through a simple algorithm, as demonstrated in Figure 2.11. This algorithm corresponds to calculating the line graph of the level space scheme and associating the line graph vertices with the starting energy of the corresponding transition.

1. Step 1: Replace all transitions in level space with vertices in transition space. Associate these vertices with the starting energy of the corresponding level space transitions.
2. Step 2: Examine each level in level space. Place directed edges from all incoming transition vertices to all outgoing transition vertices. Assign weight equal to the branching ratio of the outgoing transition.

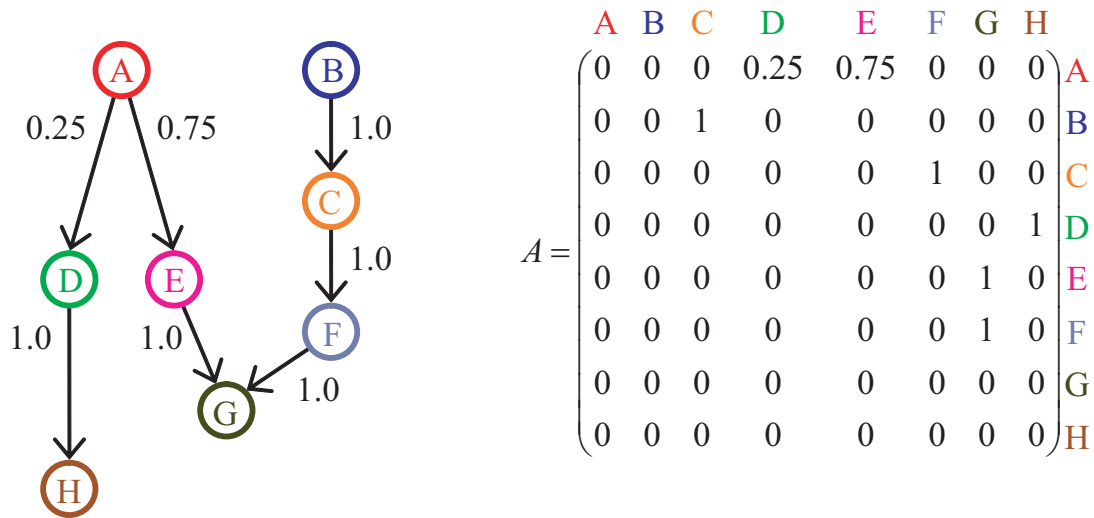


Figure 2.8: A transition space level scheme (left), and its associated transition space adjacency matrix (right). This transition space scheme corresponds to the level space scheme presented in Figure 2.6.

Unfortunately, it is far more complicated to convert schemes in transition space to level space. The added complexity derives from the abstract nature of edges in transition space. Since edges now represent more than one possibility, judgements are required to determine which possibility is correct. One way to look at the problem is that for level space to transition space conversions, each level space scheme has exactly one transition space representation, whereas each transition space scheme has an arbitrary number of level space representations.

That being said, the transformation from transition space to level space can be accomplished by gradually building up a level space scheme from the transition scheme, with periodic judgements required when apparent inconsistencies are introduced.

A number of examples of level space to transition space conversions are in appendix A, and an example of converting a transition space scheme to level space is given in appendix B.4.

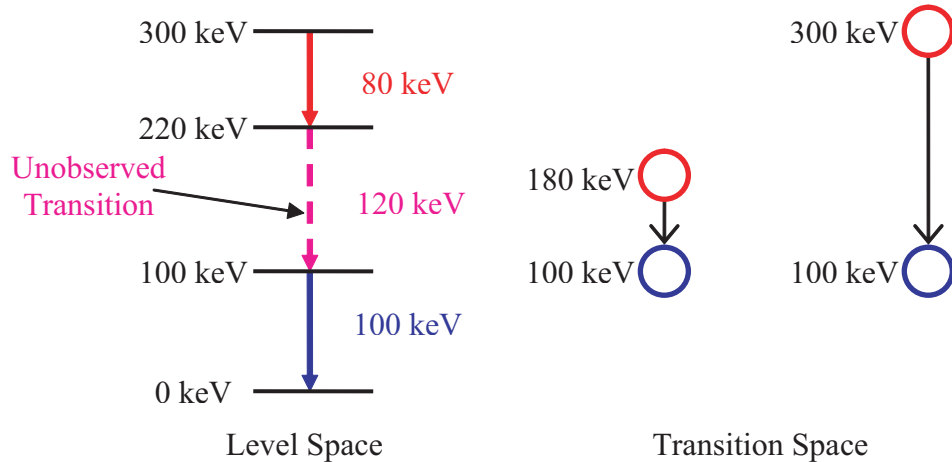


Figure 2.9: In this scheme the correct starting energy of the 80 keV transition is 300 keV. However, from the experimental data it would be concluded that it has a starting energy of 180 keV, as there is no information about the 120 keV transition.

2.2.2.2 The Abstract Nature of Edges

Edges in transition space are abstract connections between transitions. In their simplest form, an edge is a level. However, it is equally possible for an edge to represent a more complex structure.

This ambiguity creates challenges when transforming from transition space to level space as a judgement call must be made to ascertain the correct level scheme representation. However, it allows a great deal of flexibility and added freedom in level scheme creation. This added freedom is extremely useful for growing level schemes - which is the process of iteratively adding transitions to a level scheme.

Since each edge in the transition space scheme represents an abstract connection, transitions can be arbitrarily removed from a level scheme, folding the connectivity of the removed transitions into other edges, as in Figure 2.12.

From that capability, it follows that it is possible to select an arbitrary subset of the available transitions, construct a transition space level scheme, then introduce the excluded transitions one-by-one without destroying the integrity of the partial level

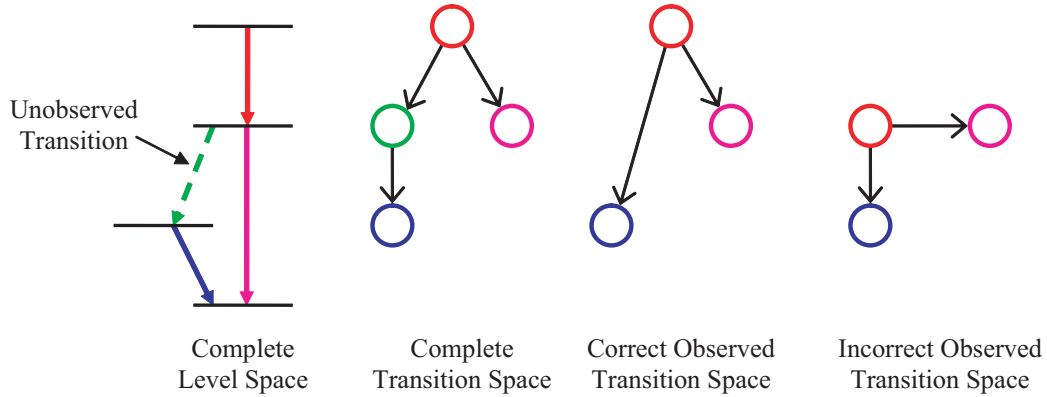


Figure 2.10: If there are two decay paths leading from a level, one of which includes an unobserved transition, the starting energy of the transition will differ depending on which path is used to calculate the starting energy. This energy mismatch can be used to locate unobserved transitions.

scheme. This is in contrast to level space schemes where it is generally only possible to add transitions at the top of the scheme without destroying the integrity of the level scheme.

Another use of the abstract nature of edges regards floating bands. Floating bands occur when the decay from a level is highly fragmented. This results in many paths from the level to a lower lying level, with each of the paths having insufficiently intensity for detection. If there is an intense transition from the lower level, a transition scheme would place edges from transitions decaying into the high energy transition to transitions decaying from the lower energy level, where the edges represent the collective effect of the intermediate transitions.

2.2.2.3 Level Identification

The state of a nucleus with a given energy does not depend on how the nucleus reached that state - in particular, the branching ratios associated with that level must be invariant. This is manifested in transition space by the requirement that if two transitions decay to a given transition, the two transitions must decay to the exactly the same transitions, with the same branching ratios. As a result, if two

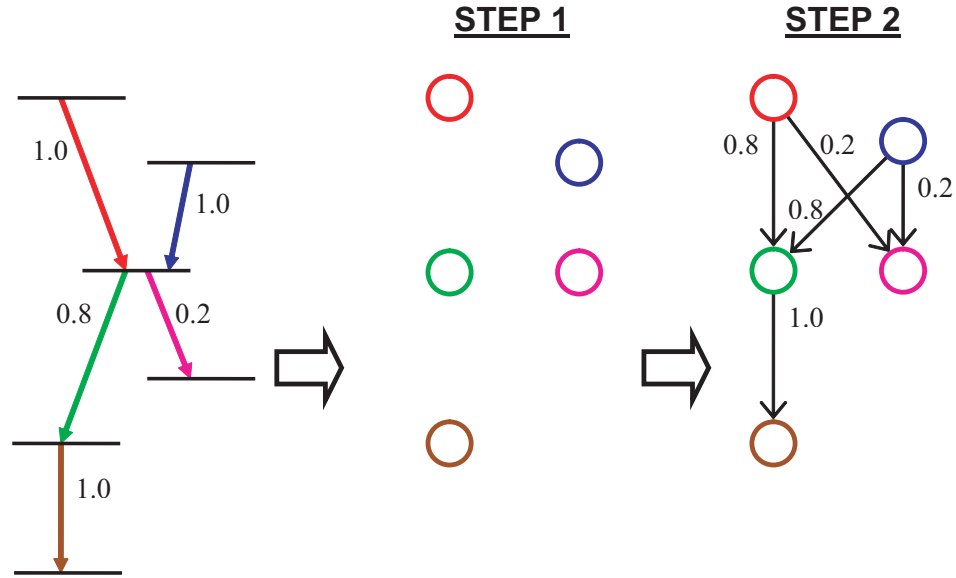


Figure 2.11: Step 1: All transitions in the scheme in level space on the left are replaced with vertices in the scheme in transition space in the centre. The vertices are placed at the energy they decay from. This means that if two transitions decay from the same level, there will be two transitions at the same energy. Step 2: Edges are placed between all ‘adjacent’ transitions. Edges are weighted by the branching ratio of the outgoing transition. Note that the top two transitions decay to the same transitions. This implies that the top two transitions decay to the same level, as per Section 2.2.2.3.

columns of the adjacency matrix share a common entry, the columns correspond to transitions that decay from the same level, and therefore the two columns must be scalar multiples of each other. Similarly, if two rows share a common entry, the rows correspond to transitions that decay to the same level, and therefore the rows must be equal.

An exception to this rule occurs when one or more of the edges involved include unobserved transitions. In this case, the edges including the unobserved transitions should be considered separately from the single-level edges.

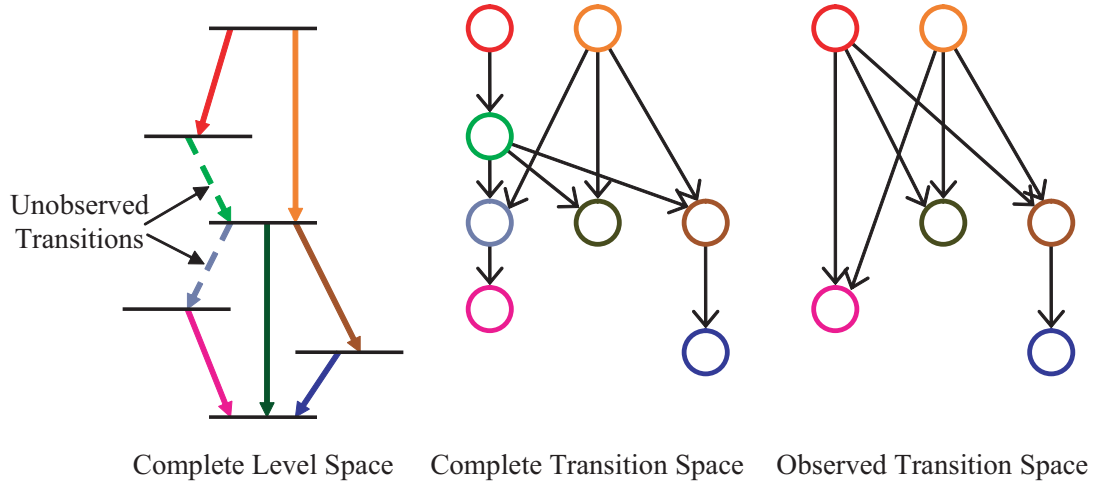


Figure 2.12: Removing transitions from a transition space causes the removed transition to become an ‘unobserved transition’, and as a result its connectivity is included in edges that connect its parent transitions to its daughter transitions. Note that this is a purely local effect.

2.2.2.4 Destination Energy Transition Space

In this section, transitions have been associated with the energy of the source level. It would be equally valid to associate transitions with the energy of the destination level. The two representations are shown in Figure 2.13.

The choice of using the source energy or the destination energy will change the appearance of the schemes, but it will not affect the underlying connectivity of the scheme. In particular, using the source energy emphasizes shared source energy levels, whereas using the destination energy emphasizes shared destination energy levels.

Since nuclear level schemes are usually constructed from the bottom up, new transitions will be added to the source energy levels of preexisting transitions. Therefore, it is generally more useful to emphasize the source energy levels. In particular, in terms of connectivity, emphasizing source levels results in it being obvious what a new transition will decay to, whereas emphasizing destination transitions emphasizes what a transition will be in anticoincidence with.

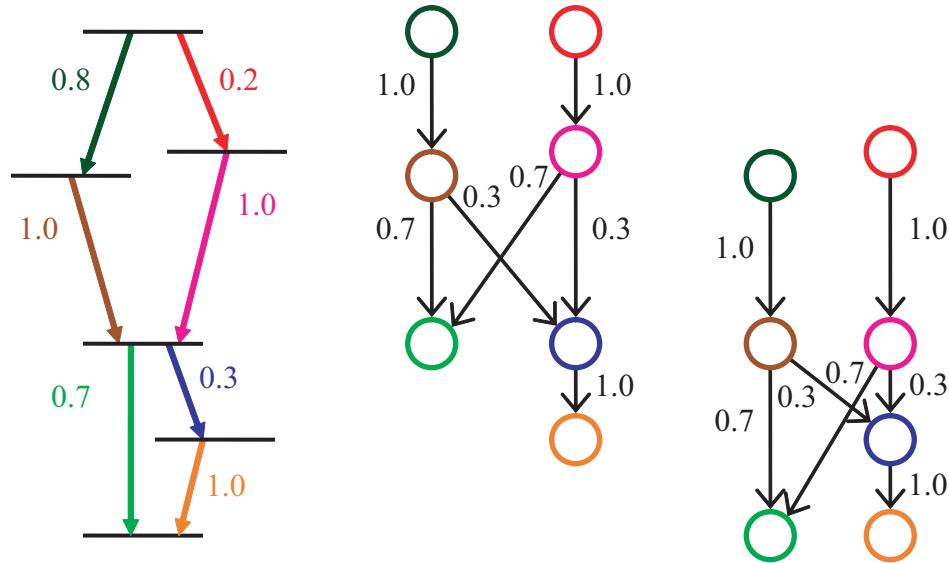


Figure 2.13: Level space scheme, source and destination representation transition schemes.

However, it is useful to look at both representations - especially when converting a transition space scheme to a level space scheme, or when searching for possible inconsistencies - since the two representations highlight different aspects of the scheme.

2.2.3 Evolutionary Algorithms

Evolutionary algorithms are a versatile method of optimization that model evolution through natural selection [7]. Their flexibility and power makes evolutionary algorithms suitable for a wide variety of problems - though they are generally outperformed by algorithms designed to solve a specific class of problem. As a result, evolutionary algorithms are an excellent tool for exploring methods of automated level scheme determination, and have been previously explored as a means to detect rotational bands in experimental data [8].

Evolutionary algorithms require a fitness function, a source of variation and a method of selecting candidate solutions for reproduction and elimination. Initially, the population of candidate solutions is seeded with a number of candidate solutions.

Natural selection, driven by a fitness function is performed on the population. The survivors reproduce, thereby regenerating the population, as depicted in Figure 2.14. Over many iterations, the population will change to favour candidate solutions with a high fitness. As a result, by selecting a fitness function that corresponds to an optimization criteria, evolutionary algorithms can be used as a method of optimization.

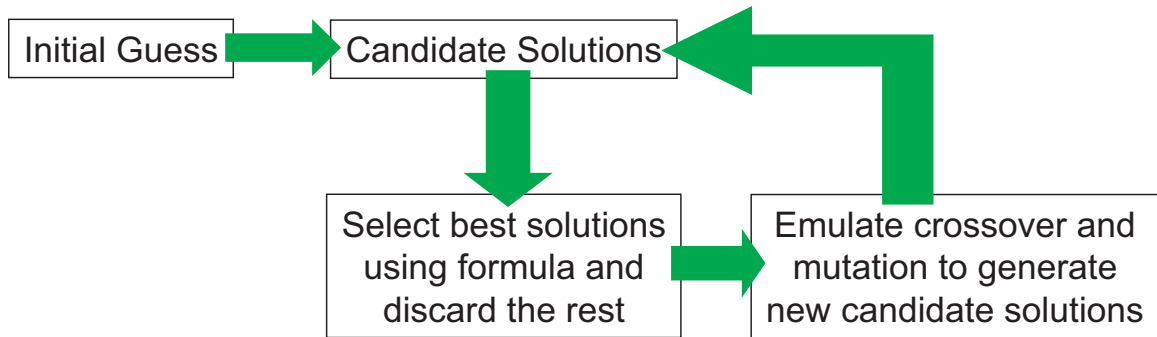


Figure 2.14: Evolutionary Algorithm Flowchart.

In order for an evolutionary algorithm to be successful its characteristics must encourage evolution. The representation of candidate solutions must ensure that similar candidate solutions have similar fitness. This allows the algorithm to progressively move towards an optima. The process of reproduction should allow both incremental improvement of solutions and drastic jumps through solution space. As a result, the process of reproduction generally consists of two sources of variation - mutation and crossover. The mutation operator is responsible for incrementally improving solutions. As a result, it should be capable of performing most conceivable small changes to the candidate solutions. The crossover operator combine aspects from multiple candidate solutions, resulting in large jumps through solution space when two dissimilar candidate solutions are combined. A method of selecting candidate solutions for crossover is shown in Figure 2.15. Ideally, crossover operators take the best aspects of the initial candidate solutions and combines them into a new superior solution. Therefore, crossover operators should faithfully reproduce the

selected characteristics in the produced solutions without destroying their structural integrity. Furthermore, as crossover operators rely on combining characteristics from dissimilar candidate solutions, it is essential for the population to be diverse. Finally, it is essential that the representation, mutation and crossover operators interact with the fitness function to encourage movement towards the global optima.

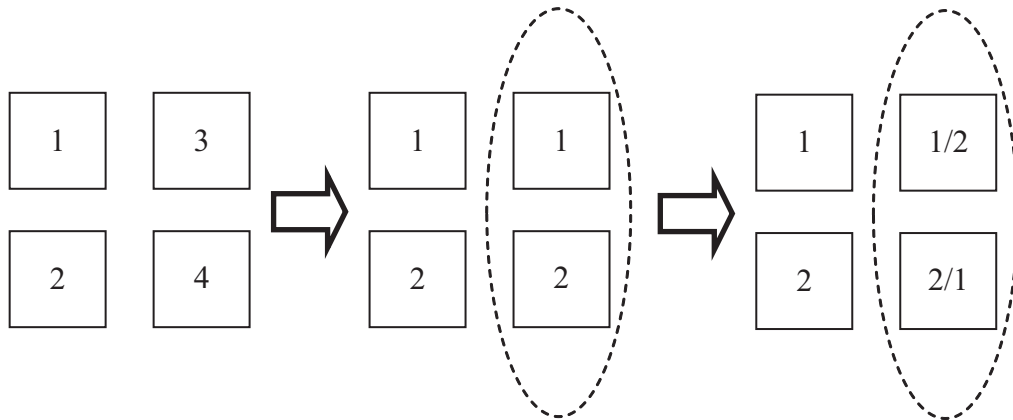


Figure 2.15: The worst two candidate solutions in a group of four are replaced by duplicates of the best two candidate solutions. Next, a crossover operator applied to the two copies, producing two new solutions that consist of a mixture of the two best solutions. Finally, a mutation operator is applied to the two new solutions

Chapter 3

Analytical Formula

3.1 Introduction

An analytical formula that directly relates experimentally measurable quantities to level schemes was developed in order to simplify the process of level scheme creation. A mathematical representation of both the experimental data and the level scheme is required for the derivation of an analytical formula.

3.2 Experimentally Measurable Quantities

In γ -ray spectroscopy experiments, the relevant experimentally measurable quantities are ‘singles spectra’ and ‘coincidence matrices’. Singles spectra are 1-dimensional histograms where each bin contains the number of γ rays detected with a specific energy. Coincidence matrices are 2-dimensional histograms with each bin containing the number of pairs of γ rays detected with the associated energy combination within a specified time window. For both singles spectra and coincidence matrices, each bin corresponds to an energy range - typically on the order of 0.5 keV.

An important experimental detail is the trigger condition for the data acquisition system. In order to record data of a given multiplicity without biasing the data,

it is necessary for the trigger condition to be set for that multiplicity (or less). For example, if coincidence data is taken (multiplicity two), singles data (multiplicity one) cannot be created by projecting the two dimensional coincidence matrix. If such a projection was performed, the resulting spectra would be biased towards transitions in long decay paths (as it is more probable for these transitions to be in coincidence with other transitions). The spectra would also lack all transitions in length one decay paths. Therefore, in theory, the trigger condition should be set to accept singles, as events with a higher multiplicity than the trigger condition will be included in the data sets. However, a problem arises in practice, as γ -ray spectrometers are typically only 1% to 20% efficient. As a result, many orders of magnitude more singles events will be observed than higher multiplicity events. The immense number of singles events will cause an unacceptably high amount of dead time in the system. Therefore, a complicated trigger that accepts scaled down singles and coincidence events must be used. The data acquisition system must also be set to flag scaled down singles events, which will be scaled up and placed in a scaled singles histogram for analysis.

There are many features in the experimental data - ranging from Compton edges to the broadening of peaks due to detector characteristics. To first order these features only serve to complicate the data, and as a result they are not included the mathematical representation of the experimental transition data. This can be accomplished by changing from an energy based binning system to a transition based binning system. Fitting all of the peaks in the singles spectra and coincidence matrices and constructing new histograms from the peak areas produces a representation where each row/column corresponds to a specific transition, rather than an energy range.

This change in representation drastically reduces the complexity of the experimental data while moving towards a more natural representation for level schemes. An important note is that in such a representation all energy information has been removed

from the histograms, and as a result the energy associated with each row/column of the matrix must be recorded separately.

3.2.1 Directed Reduced Coincidence Matrix

A reduced coincidence matrix C is a 2-dimensional matrix, where the elements are the peaks areas taken from the coincidence matrix. From an experimental standpoint, since the characteristic half life of a typical level is shorter than the detector time resolution, if two transitions are observed in coincidence, it is impossible to determine which γ ray was produced first. As a result, whenever a transition i and a transition j are observed at the same time, the entries in the matrix at $C_{i,j}$ and $C_{j,i}$ are incremented. However, since level schemes are by nature directed, it is more natural to use a directed reduced coincidence matrix. In a directed reduced coincidence matrix, if the nucleus decays through transition i into transition j , $D_{i,j}$ is incremented, but $D_{j,i}$ is not incremented. This leads to the relationship:

$$C = D + D^T. \tag{3.1}$$

Unfortunately, determining D given C is non-trivial and is one of the key issues that level scheme determination methods must face.

3.2.2 Singles Matrix

The singles matrix S is a diagonal matrix, where the diagonal elements are the peak areas taken from the singles spectra, as shown in Figure 3.1.

In the case where there are peaks in the coincidence matrix that are not observed in the singles spectrum, a reasonable estimate of the singles peak area should be used. This estimate will perturb branching ratios in the adjacency matrix but should have

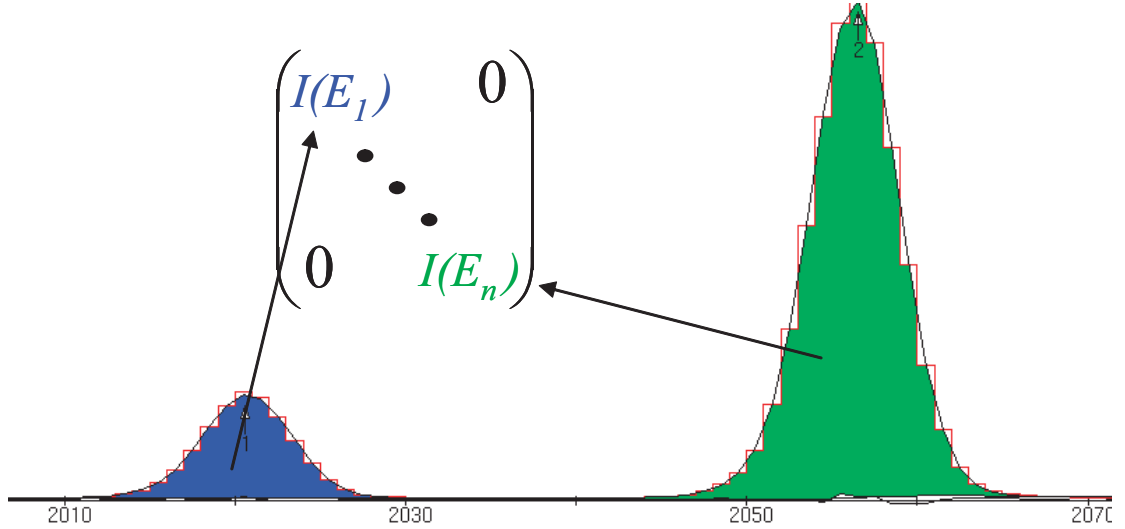


Figure 3.1: In order to construct the singles matrix, all peaks from the singles spectra are fitted, and placed as the diagonal elements of a matrix.

little effect on the structure of the level scheme. Approximations of singles intensities can be made from the coincidence matrix by examining coincidences between the transition of interest and ground state transitions. Alternatively, given an adjacency matrix and the initial population of the levels in the level scheme, the singles matrix can be calculated. This approach would be most useful for in-beam experiments where the initial population as a function of energy can be estimated provided knowledge of the level spin.

3.3 Derivation of Formula

If we consider a directed reduced coincidence matrix D , the element $D_{i,j}$ is the number of times that transition i was detected immediately prior to detecting transition j . This equals S_i , the total number of times transition i was detected, multiplied by $P_{i,j}$, the probability of detecting transition j given that transition i was observed:

$$D_{i,j} = S_i P_{i,j}. \quad (3.2)$$

However, $P_{i,j}$ is equal to the probability of decaying from transition i to transition j , and hence can be represented as an infinite sum of adjacency matrix powers, as per Equation (2.1), giving:

$$D_{i,j} = S_i(A + A^2 + A^3 + \dots)_{i,j}. \quad (3.3)$$

Since S is a diagonal matrix, this implies that:

$$D = S(A + A^2 + A^3 + \dots). \quad (3.4)$$

Using Equation (2.3) we can rewrite it as:

$$D = S((I - A)^{-1} - I), \quad (3.5)$$

from which we can solve for A :

$$A = I - (S^{-1}D + I)^{-1}. \quad (3.6)$$

Equation (3.6) directly relates level scheme structure to experiment through singles intensities and directed coincidence data.

3.4 Discussion

The approach of directly relating level schemes to experimental intensities differs significantly from most other approaches to level scheme construction, as it is entirely based on the flow of intensity through a level scheme and uses a formula to directly calculate the level scheme. Additionally, the scheme that it calculates may not be physically possible, as it is calculated solely from intensities and does not contain any information about transition energies or nuclear physics. However, the scheme that

it produces should be ‘close’ to the true scheme, and will emphasize different aspects of the experimental data than other techniques.

Due to the intensity based nature of this method, it will be most useful for solving level schemes with a reasonable number of cross-band transitions. These cross-band transitions provide a significant amount of extra information to this method. On the other hand, it will be less useful for solving level schemes with long cascades of transitions and with few cross transitions, as there will be little information about the transition ordering. Furthermore there are efficient methods for solving such schemes manually.

An important feature of this formula is that it does not differentiate between positive and negative intensity transitions - it will use whatever is required for the matrix inversion. Since negative intensity transitions are non-physical, their presence can be used to check the validity of the produced level schemes, and as a signature for doublets (doublets violate the assumptions, and hence should produce non-physical results).

3.5 Applications

The ability to directly relate experimentally measurable quantities to a level scheme is a very powerful tool, with applications of checking pre-existing level schemes and of solving directly for level schemes from experimental data.

The more interesting use is solving directly for level schemes. This is straightforward in the case that a directed reduced coincidence matrix that includes all transitions of interest exists. Unfortunately, there are a number of challenges that must be overcome before using this method on real experimental data. In short these challenges are:

1. Experiments allow the construction of coincidence matrices, not directed co-

incidence matrices - it is trivial to calculate C from D as per Equation (3.1). However calculating D from C has a huge number of solutions, and physics knowledge must be used to select the correct solution.

2. Coincidence matrices may be missing transitions of interest - there may be low-energy and low-intensity transitions that are not detected. This will affect the connectivity of a level scheme, likely affecting energy conservation.
3. The derivation implicitly assumes that each row/column corresponds to a single transition. This assumption is violated in the case of irresolvable doublets.
4. Physicists are interested in level space level schemes, not transition space level schemes, thereby requiring an efficient and accurate method of transforming from transition space to level space.

On the other hand it is technically straightforward to use Equation (3.6) to verify pre-existing level schemes as it bypasses all of the challenges associated with directly solving for level schemes.

3.5.1 Doublets

An implicit assumption made in this representation is that each peak in the singles spectrum and coincidence matrix corresponds to a single transition. However, there are often irresolvable doublets in the experimental data. These doublets effectively cause two transitions to be represented as one transition in the transition space level scheme. Unsurprisingly this is somewhat of a problem - particularly with respect to energy conservation, but also for level identification. Fortunately, doublets have a characteristic signature that makes them easy to identify. By representing two transitions as one, false coincidences are introduced between transitions feeding the first transition and decaying from the second transition. In order to compensate for

this, negative ‘cross’ transitions are added that exactly cancel the false transition, as in Figure 3.2. This pattern of perfectly balanced false coincidences is an excellent signature for detecting doublets. This signature can be viewed as adding features to the A term of Equation (3.4) to correct for contributions from the A^2 term resulting from representing two transitions as one. For the case where the two transitions are in different decay paths this correction will be exact. However, if the two transitions are in the same decay path, the effects of higher order terms will perturb the signature.

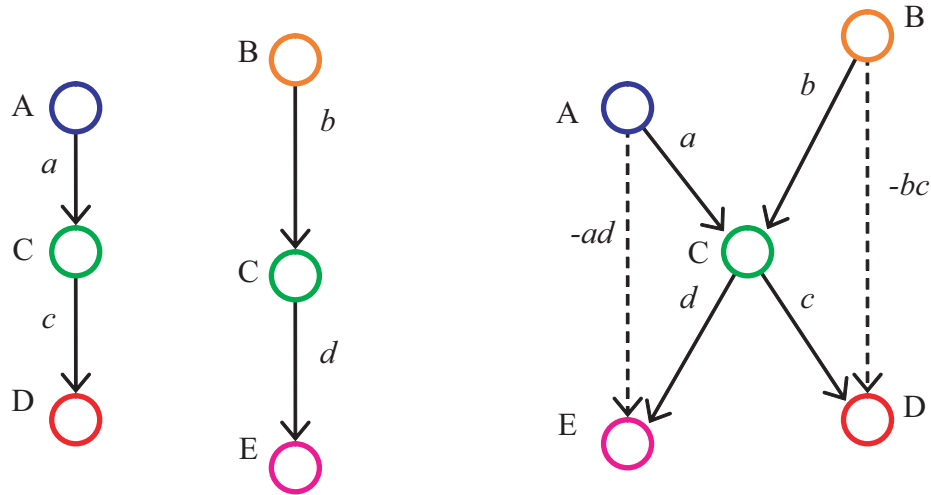


Figure 3.2: Representing the doublet transitions C as one transition introduces false coincidences between transitions A and E and between transitions B and D. Negative ‘cross’ transitions are introduced to cancel these false coincidence.

Chapter 4

Formula Based Approaches

4.1 Introduction

One of the simplest possible methods of level scheme determination would be through the use of a formula. In an attempt to realize this goal, two formulaic approaches were developed. The first approach uses Equation (3.6) to directly solve for the adjacency matrix from the singles matrix and the directed coincidence matrix. This approach produces excellent results for simulated data. However, it cannot be used on experimental data, as the directed coincidence matrix is not experimentally measurable. The second approach combines Equation (3.6) with Equation (3.1) in order to derive a self-consistent equation that uses the singles matrix and the coincidence matrix - both of which are experimentally measurable. The self-consistent approach works for extremely small levels schemes (6 levels and 10 transitions), but fails dismally for larger level schemes.

4.2 Direct Analytical Solution

4.2.1 Introduction

Equation (3.6), derived in Section 3.3, directly relates level schemes to directed experimental data. It would be highly desirable to use Equation (3.6) to directly solve for level schemes from undirected experimental data. However, before its applicability to undirected data can be investigated, it is essential to understand its strengths and limitations, which can be investigated through the use of simulated directed data.

In this section, simulated directed data were used to verify that Equation (3.6) is capable of solving directly for level schemes in the presence and absence of irresolvable doublets. In addition, the sensitivity of Equation (3.6) to Poisson distributed errors in the singles and coincidence matrices was investigated.

It was found that Equation (3.6) worked essentially perfectly in all situations, using trivial amounts of computational time.

4.2.2 Methodology

4.2.2.1 Data Simulation

Simulated data were used to test the validity of Equation (3.6) and subsequently to investigate different methods of automated level scheme determination. The data were produced by creating random level schemes, and calculating the expected directed reduced coincidence matrices, reduced coincidence matrices, and singles matrices from them. Poisson distributed errors were incorporated into the intensities of the elements in these matrices. Errors were calculated for ten million nuclei decaying through the scheme, distributed according to the ‘starting counts’ of each level. The transition energy associated with the various rows/columns was also tracked.

Random level schemes, such as the one depicted in Figure 4.1 were produced using the following algorithm:

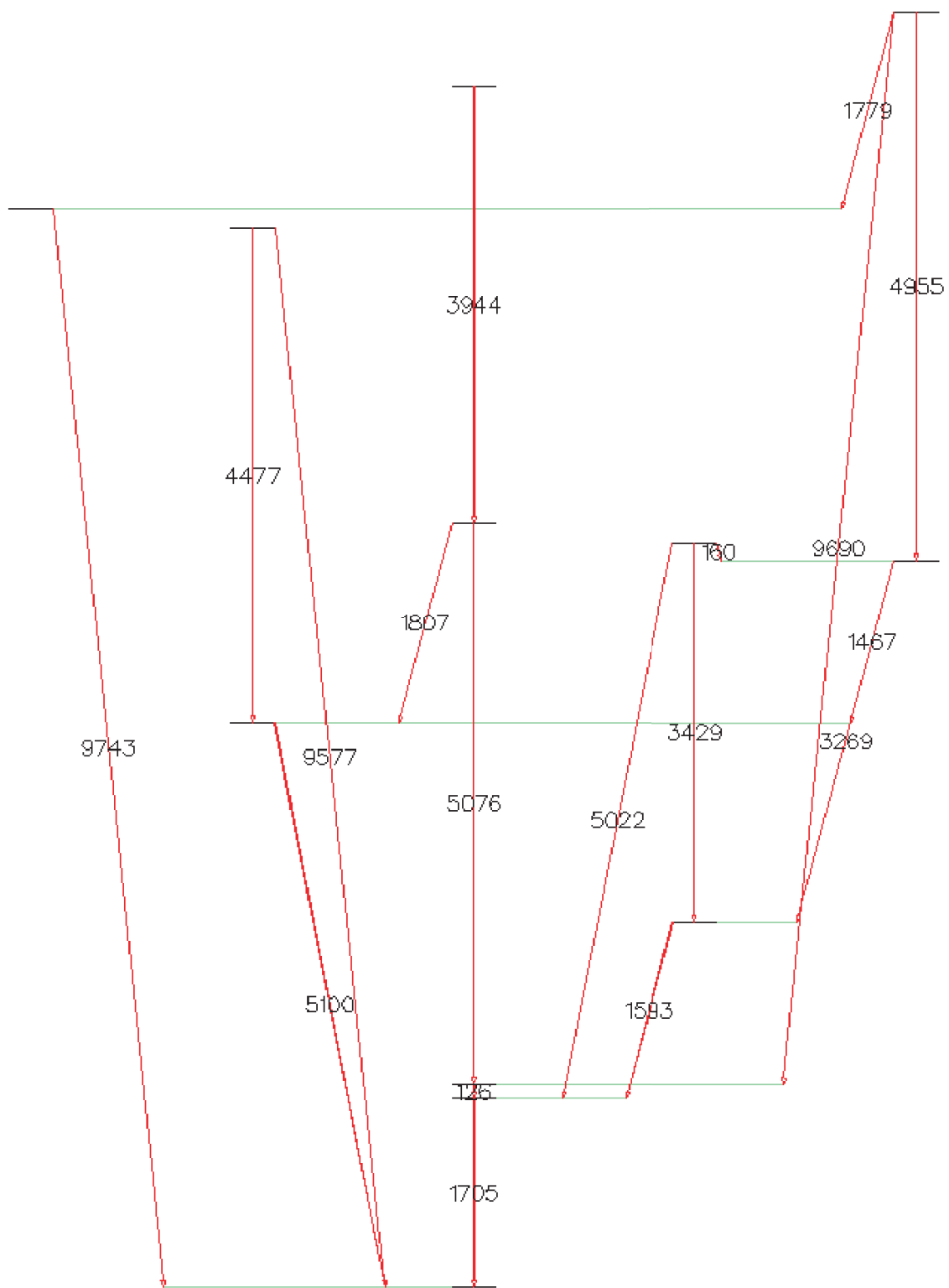


Figure 4.1: A randomly generated level scheme with 12 levels and 18 transitions.

1. Assign random energies to the levels. Shift the levels such that the lowest energy level is at 0 keV.
2. For each irresolvable doublet to be included, place two transitions. Change energies of levels such that the doublet transitions have the same energy.
3. Place one transition decaying from all levels, excluding the ground state. If this transition duplicates an already placed transition (i.e. it is a doublet transition), then instead place an extra transition in step 4.
4. Place all remaining transitions randomly, without duplicating any transitions.
5. Assign random ‘starting counts’ to each non-ground state level. (Simulating decays into the level scheme.)
6. Assign random branching ratios.

Transitions were placed by randomly selecting two levels, and placing a transition from the higher energy level to the lower energy level. This method of level scheme generation does not incorporate any band structure or spin into the level scheme. As a result, the produced level schemes are a simplified version of experimental level schemes.

After the scheme is created, and the matrices are calculated, the rows/columns of the matrices corresponding to irresolvable doublets are combined.

4.2.2.2 Calculations

The transition space adjacency matrix for the level scheme was calculated using Equation (3.6), the simulated directed reduced coincidence matrix, and the singles matrix. The resulting adjacency matrix was converted to a level space level scheme using the list of transition energies, as per appendix B.

Calculations were performed on a wide range of level schemes, ranging in size from 10 transitions and 6 levels up to 450 transitions and 270 levels. Calculation times ranged from 0.01 seconds to 3.2 seconds.

4.2.3 Results

Applying Equation (3.6) to simulated directed data was extremely successful. Correct level schemes were produced in all cases tested. Poisson distributed errors had no effect on the produced level schemes and irresolvable doublets produced the expected characteristic signatures, as discussed in Section 3.5.1.

These results demonstrate that Equation (3.6) is fast, accurate and robust. As a result, it is reasonable to use Equation (3.6) as a basis for determining level schemes from undirected data. Ideally, combining a different approach with Equation (3.6) will allow its applicability to be extended from directed data to undirected data, while preserving its speed and accuracy.

4.3 Iterative Self-Consistent Solution

4.3.1 Introduction

A logical approach to the undirected nature of experimental data is to derive a formula, similar to Equation (3.6) that utilizes undirected data. Combining (3.1) with (3.5) leads to the derivation of a self-consistent formula that directly relates a level scheme to undirected experimental data. However, the use of (3.1) introduces a huge number of additional solutions, thereby necessitating the use of additional criteria in order for the self-consistent equation to converge to the desired solution. While it may be possible to devise such criteria, all criteria tested failed for level schemes larger than 10 transitions and 6 levels.

4.3.1.1 Derivation

Combining equations (3.5) and (3.1) gives:

$$C = D + D^T = S((I - A)^{-1} - I) + (S((I - A)^{-1} - I))^T, \quad (4.1)$$

which simplifies to:

$$C = S((I - A)^{-1} - I) + ((I - A^T)^{-1} - I)S. \quad (4.2)$$

Equation (4.2) directly relates the experimentally measurable quantities of C and S to the level scheme through A . This equation can be solved self-consistently for A .

4.3.1.2 Solution Space

Using Equation (3.1) in the course of the derivation has the effect of greatly increasing the number of solutions. Instead of having a unique solution, Equation (4.2) has one solution for each of the infinitely many D matrices that could produce C . As a result, in order to use the self-consistent equation, a method of converging to the solution associated with the correct D is required.

Additionally, it is possible, though unlikely for non-trivial level schemes, that an experimental data set could correspond to two physical level schemes, depending on how the coincidence matrix C was decomposed into the directed coincidence matrix D . In this case, additional information could be used to determine the correct level scheme.

4.3.2 Methodology

The self-consistent equation derived in Section 4.3.1.1 was used in combination with the criteria in Section 4.3.2.1 to determine level schemes. Simulated data were pro-

duced as per Section 4.2.2.1.

The starting point used for the adjacency matrix in the self-consistent equation was a 0 matrix.

4.3.2.1 Convergence Criteria

In order for an iterative self-consistent equation to be useful, it must converge to the correct solution. Therefore, one or more convergence criteria must be applied. Ideally, these criteria would cause the algorithm to move through the solutions of Equation (4.2) towards the physical solution. One challenge for the development of such criteria is that it is difficult to visualize the set of solutions, and to understand the effects of various convergence criteria.

In abstract terms, convergence criteria rely on extra information that is not incorporated into the self-consistent equation to determine the correct solution. In the case of level schemes, physical constraints provide a significant amount of additional information. In particular, energy conservation, continuity of flow, and the Markov property (evolution from a given state is independent of past states) must be satisfied. Of these constraints, energy conservation is the most powerful, though the other constraints provide important supplementary information.

If the convergence criteria used was ‘does the scheme satisfy energy conservation, continuity of flow, and the Markov property’, and the self-consistent equation converged, it would converge to a physical (and likely correct) solution. Unfortunately, this is not practical for two reasons. Firstly, it is difficult to determine that the three conditions are satisfied if there is any uncertainty in the system. Secondly, it would be very challenging to devise an algorithm that modified a level scheme such that it obeyed the three conditions without destroying the structure of the level scheme. (Destroying the level scheme structure would make convergence difficult.) As a result, it is impractical to directly base convergence criteria on these conditions.

One approach to this problem is to examine the conditions and create loose criteria based on their implications. These loose criteria will be much simpler to implement, and can be designed such that level schemes can be modified to satisfy them, without destroying their fundamental structure.

An added complication is that the presence of irresolvable doublets or the existence of unobserved transitions will destroy energy conservation and the Markov property, if they are not properly taken into account.

It was found that the use of almost any criteria would cause the algorithm to converge to a solution in solution space. Unfortunately, all of the investigated criteria caused the algorithm to converge to non-physical solutions for level schemes larger than 10 transitions and 6 levels.

The following criteria (and combinations of them) were investigated:

1. Each iteration, set A_n to $\frac{A_{n-1} + A_{n-1}^T}{2}$.
2. Each iteration, set all negative intensity elements of A to zero.
3. Each iteration, if $A_{i,j} > A_{j,i}$, set $A_{j,i} = 0$.
4. Each iteration, if $|A_{i,j}| > |A_{j,i}|$, set $A_{j,i} = 0$.

The first criteria increases the rate of convergence, as it eliminates large erratic changes in the adjacency matrix. The second criteria follows from how nuclei decay through a level scheme - there cannot be negative intensity transitions (follows from continuity of flow). The third and fourth criteria follow from conservation of energy. Specifically, if a transition i decays to a transition j , transition i must have a higher starting energy than j . Therefore, a transition decaying from j to i would be non-physical, as decays must decrease the energy in the system.

The best results for non-trivial schemes were achieved when the first, second and third criteria were combined. However, for schemes larger than 10 transitions

and 6 levels, the self-consistent equation converged to incorrect solutions, where the adjacency matrices showed some similarities to the correct adjacency matrices.

It is probable that these criteria failed because they do not take into account the transitive nature of energy conservation - specifically, if transition i decays to transition j , and transition j decays to transition k , then transition k cannot decay to transition i . As a result, when decay chains of length three or longer become common (i.e. beyond 10 transitions), the criteria are insufficiently selective. It would be possible to devise criteria that incorporate the transitive nature of energy conservation, but this leads to the problems associated with implementing a complete check of energy conservation, continuity of flow, and the Markov property.

It is also important for convergence criteria to function properly in the presence of doublets. The second and third criteria fail in the presence of doublets, as they conflict with the characteristic negative ‘cross’ transitions associated with doublets, as discussed in Section 3.5.1.

4.3.3 Results

While a self-consistent approach to determining level schemes would be very attractive, this approach failed for level schemes larger than 10 transitions and 6 levels. It may be possible to develop convergence criteria that would allow this method to solve moderately sized simulated level schemes, however it would be very difficult to apply it to large experimental data sets containing irresolvable doublets.

Chapter 5

Evolutionary Approaches

5.1 Introduction

Determining nuclear level schemes from experimental data can be formulated as the optimization problem of locating a level scheme that best reproduces a set of experimental data. In this formulation, an optimization criteria (or fitness function) and a level scheme representation are required. Ideally, the optimization criteria will be an accurate measure of how close a given level scheme is to the correct level scheme. As a result, it should take into account several ideas - specifically how accurately the level scheme reproduces the experimental data, and how physically realistic the level scheme is. These ideas are very complex, and it is difficult to create an optimization criteria that incorporates all of the available information. A level scheme representation is also required. While representations can be viewed merely as an interpretation of level schemes, their structure has an enormous effect on the implementation of the optimization problem, and as a result on the difficulty of locating the correct solution.

Evolutionary algorithms are an extremely flexible method of optimization. Their flexibility arises from their lack of dependence on the data representation. They can be used on any data where a representation, a fitness function (optimization criteria),

and methods of creating new candidate solutions from pre-existing candidate solutions can be formulated. As a result, evolutionary algorithms are well suited for optimizing level schemes

Three possible representations were investigated in the course of this work with varying degrees of success. In the first representation, level schemes were depicted as directed graphs, with energy levels represented as vertices, and transitions represented as edges. This representation parallels the traditional view of level schemes, and as a result it is a very natural space to work in - though it lacks the flexibility of more abstract spaces. Results for this representation were promising, including successful solutions of level schemes with up to 50 transitions and 30 levels from simulated data. However, these results required supplementary algorithms. Furthermore, this representation may have difficulties with the complexities introduced by the use of experimental data, in part due to its non-abstract nature. As a result, while this approach shows promise, research shifted to more abstract avenues upon the derivation of Equation (3.6).

For the second representation, level schemes were again represented as directed graphs, except the transitions were represented as vertices and the energy levels (or abstract connections between transitions) were represented as edges. This representation matches the form of the experimental data, and incorporates Equation (3.6). Through the use of this representation, level schemes with 10 transitions and 6 levels were calculated. The development of this representation suffers from the simplicity of the mutation and crossover operators. Development of complicated mutation and crossover operators may greatly improve the results produced by this representation. However, said development would require significant improvements in automated transition space to level space conversion algorithms - especially for transition space schemes that do not directly correspond to a specific level space scheme (due to doublets, non-physical aspects of the transition space scheme, or missing transitions).

The third representation is a significant departure from the first two representations. In this representation, level schemes were stored as an energy ordered list of transitions. This list is used to convert the expected undirected coincidence matrix to a directed coincidence matrix. From the directed coincidence matrix, the level scheme can be directly calculated using Equation (3.6). This representation allows the use of Equation (3.6) in its most powerful form, while closely resembling the form of the experimental data. Excellent results were produced using this representation, with correct results for level schemes with 150 transitions and 60 levels. Continued optimization, in combination with longer run times will increase the power of this approach. Furthermore, these results were obtained with a very simple and straightforward method. As a result, it should be possible to resolve the complications associated with experimental data by introducing complexities into the algorithm.

5.2 Graphs in Level Space

5.2.1 Introduction

In the first representation, level schemes were presented as directed graphs in level space. This is a very common representation for level schemes. Its primary advantage is that it is very straightforward to work with. However, it is a very concrete representation, and as a result it lacks the flexibility required to accommodate unobserved transitions easily. Furthermore, as this representation focuses on energy levels rather than transitions, it is in a different space than the experimental data.

Simulated level schemes with up to 50 transitions and 30 levels were solved in the context of this representation. However, producing these results required the use of supplementary algorithms and complex mutations, and as a result this representation is likely to encounter difficulties with experimental data.

5.2.2 Methodology

5.2.2.1 Representation

Level schemes were represented as arbitrary graphs with a specified number of vertices (energy levels) and edges (transitions). Transitions in the graphs were given a specific energy, taken from the simulated data. Each level had a varying number of ‘starting counts’. Each transition had a branching ratio, with the branching ratios leaving each level normalized to one. The energies of the levels were calculated from the transition energies using a greedy algorithm (an algorithm that only uses local information). This greedy algorithm started from a presumed ground state (the level with the lowest energy in the previous iteration of the algorithm), and traversed the scheme using the most intense transitions first, setting level energies when a level was first reached. Energy conservation was not enforced by the structure of the representation. Instead, level schemes that violated energy conservation were penalized by the fitness function. This approach facilitates convergence, since the ‘shortest path’ between local optima often travels through level schemes where energy is not conserved. In addition, this approach simplifies the algorithm, as it would be difficult to create a flexible representation that enforces energy conservation. An example level scheme is presented in Figure 5.1.

5.2.2.2 Fitness Function

The fitness function consisted of two parts. The first part compared the expected coincidence matrix and the simulated coincidence matrix. The second part consisted of penalizing level schemes that violated energy conservation proportionally to the degree of energy conservation violation.

There were two methods used for comparing the two coincidence matrices. The initial method consisted of taking the squared difference on an element-by-element

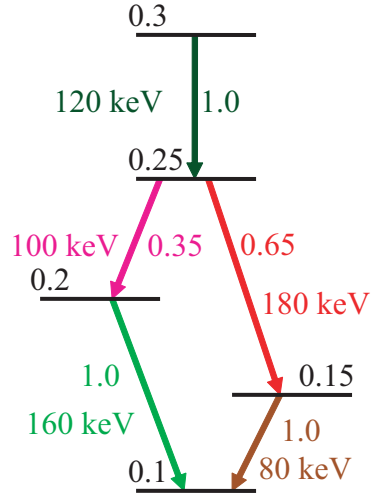


Figure 5.1: A level scheme in the level space representation. Each transition is associated with a branching ratio and an energy. Each level is assigned a number of starting counts. Level energies can be calculated from the connectivity of the level scheme and the transition energies.

basis between the expected coincidence matrix and the experimental coincidence matrix. It would be possible to instead use the absolute value of any positive power of the element-by-element difference between the two matrices, including non-integer powers. Increasing the power increases the relative sensitivity to large errors, while decreasing the power increases the relative sensitivity to small errors.

The second method treated all elements in the two matrices as either present or not-present, and penalized mismatches. Using this method allows intensities to be ignored, greatly reducing the size of the solution space.

The energy conservation component of the fitness function consisted of two parts. The first part penalized solutions based on the standard deviation of possible energies for the levels. For each level, the standard deviation of the expected energy was calculated by examining the energy of the level according to each of the incoming and outgoing transitions, with the assumption that the energy of the source/destination level of the transition was correct, as shown in Figure 5.2. The second part penalized especially bad instances of energy conservation violation. In particular, if there was

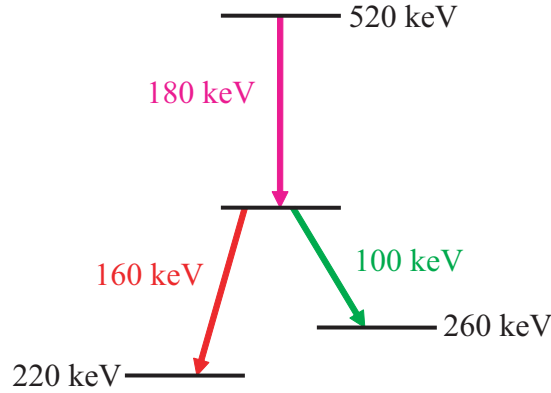


Figure 5.2: For the above level scheme, the energy of the middle level would be calculated by averaging the three possible energies, producing a value of 360 keV, with a standard deviation of 16 keV.

a transition from level A to level B, there could not be a transition from level B to level A, and there could not be two transitions both going from level A to level B.

The fitness function contributions from the coincidence matrix and the energy combinations were weighted, then summed to form the optimization criteria. The optimal weighting varied with level scheme size, and the most successful weighting factors yielded equal contributions from both parts to the fitness function. The relative size of the contributions varied with proximity of the trial level scheme to the optimum scheme, and as a result the weightings were varied as a function of iteration number.

In general, at the start of a run, the energy conservation contribution would strongly dominate. This produced a strong selection for any scheme that did not violate energy conservation, and the offspring of a few of the initial candidate solutions would quickly come to dominate, greatly reducing the diversity. It would be better if the initial candidate solutions were all reasonably fit according to the energy criteria. This could be accomplished by breaking the problem into two phases. The first phase would consist of repeatedly performing the first 100 iterations of the problem. The best solutions from this phase would then be used as the initial candidate solutions

for a full run of the algorithm.

After the energy conservation dominating phase, there is typically a period where both contributions have approximately equal effect. It is essential that the weightings are set such that this phase persists until the candidate solutions are close to the correct result. Finally, after the candidate solutions are extremely close to the optimal result, any energy violation will eliminate the organism, causing the fitness to be solely determined by the comparison of the expected and simulated coincidence matrices.

5.2.2.3 Mutation Operator

The mutation operator consisted of performing between one and five mutations (determined uniformly at random) to the candidate solution.

The following mutations were used:

- Modifying transition branching ratios.
- Modifying the starting counts of a level.
- Changing a transition destination.
- Changing a transition source.
- Swapping the source and destination of a transition.
- Merging two levels, and creating a new isolated level. An example of merging levels is shown in Figure 5.3.
- Swapping the source and destination of two transitions.
- Inserting a transition into a band (either above or below another transition).
- Swapping a transition with the transition below it.

Branching ratios were renormalized to one whenever affected by mutations. An example of moving a transition is presented in 5.4.

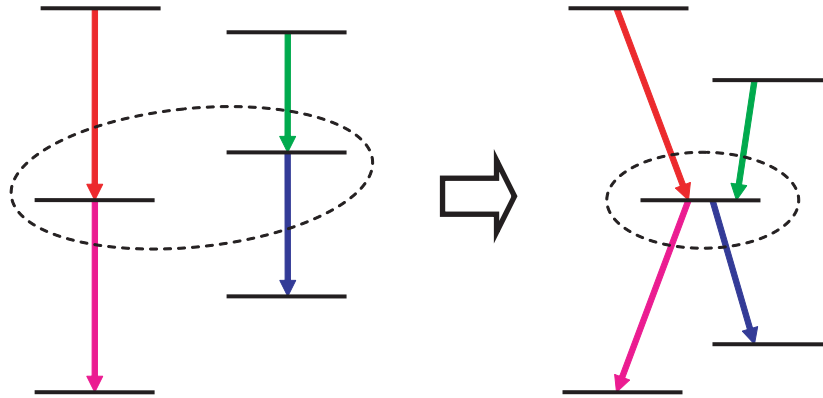


Figure 5.3: An example of the merging levels mutation operator.

5.2.2.4 Crossover Operator

The crossover operator consisted of taking two level schemes, selecting half of the transitions (by transition energy), swapping the selected transitions between the two schemes, then renormalizing branching ratios. However, due to the nature of the representation it is difficult to identify equivalent levels between level schemes. As a result, the level number (which does not relate to the structure of the level scheme) was used to identify equivalent levels. This is an imperfect method, though for candidate solutions that share a ‘common ancestor’ level number will be partially associated with equivalent levels.

5.2.2.5 Hill Climbing

Hill climbing algorithms are an excellent complement to evolutionary algorithms. A hill climbing algorithm takes a candidate solution and locates the nearest local optimum. When combined with an evolutionary algorithm, the evolutionary algorithm moves solutions between basins of attraction for different local minima, while the hill climbing algorithm converges to the actual minimum.

A Lamarckian mutation [7] consisting of searching for the local optima by repeatedly moving single transitions was applied to the fittest candidate solution every 100

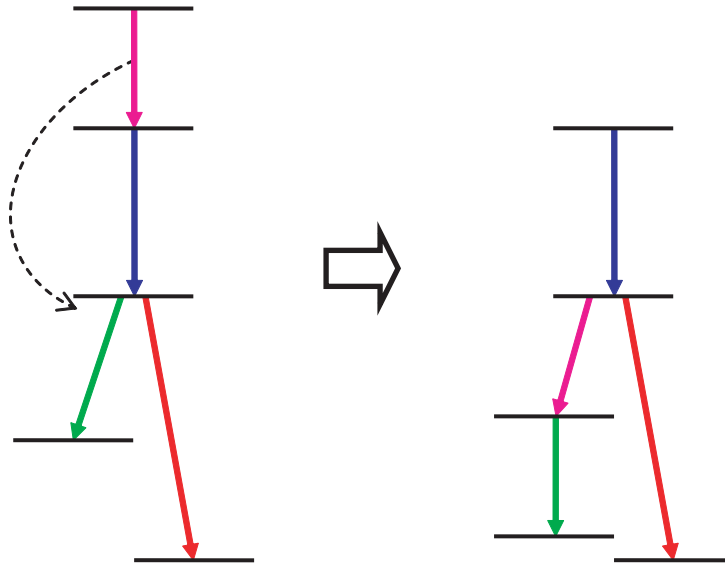


Figure 5.4: An example of the transition moving mutation operator.

iterations. While this algorithm will converge to the local optima, it is very inefficient for large level schemes. Modifying the algorithm to focus on transitions with large discrepancies between the actual and simulated coincidence matrices, and to only search a subset of nearby solutions would increase the efficiency of the hill climbing algorithm.

5.2.2.6 Growing The Level Scheme

Level schemes containing a subset of the transitions should have the same general structure as the full level scheme. As a result it is useful to start with a small number of transitions and slowly increase the number of transitions involved in the calculation. Optimization began with only the ten most intense transitions according to the singles matrix in the level scheme. Subsequent transitions were added to the level scheme by increasing the dimension of the adjacency matrix and adding an additional transition to the level scheme representations. The remaining transitions were added one-by-one with order determined by the intensity of the transitions, with a transition added every 300 iterations.

Level space representation is very amendable to adding new transitions to the top of a level scheme. Since transition intensity generally decreases for transitions associated with higher energy levels, most of the added transitions appeared at the top of the scheme. Unfortunately, due to the strong dependence on conservation of energy for the level space representation, it is far more difficult to insert new transitions into the lower regions of the scheme, and the absence of low energy transitions also inhibits the formation of correct sub-level schemes.

5.2.2.7 Intensity Fitting

Initially, the branching ratios and starting counts were free parameters. It was found that fitting these parameters using the CURFIT algorithm [9], greatly reduced the solution space and decreased overall program run time (even though intensity fitting was a slow process). It was subsequently found that changing the fitness function to only depend on the presence or absence of coincidences provided a huge improvement boost (since intensity fitting was no longer required). However, after converging close to the solution, reintroducing the intensities with fitting allows for fine tuning.

5.2.3 Difficulties

The largest difficulties encountered were the sheer size of the solution space, and the difficulty of understanding the structure of the solution space. The solution space is extremely large - given n transitions and m energy levels there are $(2 \cdot \binom{m}{2})^n$ possible graphs. For each of these graphs, the ‘starting counts’ and branching ratios can be set freely. To make matters worse, the correct number of energy levels is unknown, thereby increasing the size of solution space even further.

5.2.3.1 Doublets

While the presence of γ -ray doublets was not explicitly tested, this representation does not assume that there are no doublets. As a result, it would be possible to add doublets without destroying the fundamental structure of the representation, though this would greatly increase the search space. However, it would be necessary to specify which transitions are doublets, and how many instances of each transition exist, or add functionality for detecting doublets. Unfortunately, it would likely be difficult to write accurate doublet detection algorithms, especially when their presence is often only known at the later stages of level scheme construction.

5.2.4 Results

Good results were obtained for errorless simulated level schemes, with no γ -ray doublets present, for on the order of 30 levels and 50 transitions. The results suggested that the size of the level scheme calculated could be significantly increased successfully. Unfortunately, the current implementation of this approach scaled poorly, largely due to the hill climbing algorithm and the size of the solution space. Modifying the hill climbing algorithm as discussed in Section 5.2.2.5 and calculating the expected coincidence matrix using Equation (3.1) would provide a substantial speed increase. However, the concrete nature of this representation is likely to have difficulties adapting to complications introduced by experimental data - especially since this representation requires a large number of mutation operators, a growing level scheme and a hill climbing algorithm for simulated data. While it is probable that reasonably large schemes could be solved using this method, the development of Equation (3.5) suggested that transition space approaches were more promising. As a result, this line of investigation was abandoned in favour of the following transition space approach.

5.3 Transition Space Approach

5.3.1 Introduction

The second data representation explored was that of directed graphs in transition space. In this representation, vertices were associated with transitions, and edges were associated with abstract connections between transitions (the simplest such connection is an energy level). The graphs were stored as adjacency matrices. This representation has two advantages. Firstly, Equation (3.6) is used to quickly and accurately calculate expected coincidence matrices. Secondly, it is possible to work directly with the connectivity of the level scheme. However, these advantages are accompanied by the challenge of working in a more abstract space. Additionally, the possible solution space for this representation is immense, as it consists of the set of directed graphs with a number of vertices equal to the number of transitions in the level scheme - though the vast majority of possible graphs do not correspond to physical level schemes.

Using this representation level schemes with 10 transitions and 6 levels were determined. This method worked for small schemes, but further improvements would require the creation of complicated mutation operators. However, developing complicated mutation operators would require large improvements in automated transition space to level space conversion algorithms.

5.3.2 Methodology

5.3.2.1 Mutations

In this representation, only one mutation was used. This mutation consisted of randomly changing an entry in the adjacency matrix. Due to the representation, any change to the level scheme could be accomplished in this fashion. However, since elements are changed one-by-one, it is difficult to accomplish complex changes if the

intermediate schemes are less fit than the initial and final level schemes.

It would be possible to implement additional more complex mutations. For example it would be possible to couple changes to transitions that decay to the same level - though this would require a somewhat robust condition for determining if two transitions decay to a specific level. The development of this condition would necessitate substantial improvements in automated transition space to level space algorithms - which is a difficult, especially for transition space schemes that incorporate doublets, unobserved transitions or non-physical aspects.

5.3.2.2 Crossover

The crossover operator consisted of selecting a random set of transitions, and swapping the associated rows in the adjacency matrices. This has the effect of swapping the transition positions between the two level schemes.

5.3.3 Fitness Testing

Similarly to the level space representation, the fitness function consisted of comparing the expected and experimental coincidence matrices, and checking energy conservation. The squared element-by-element differences between the coincidence matrices was used as the first part of the fitness function, as in Section 5.2.2.2.

The energy conservation component of the fitness function consisted of three parts. The first part consisted of the standard deviation of the expected transition energies, parallel to the method used in the level space representation, as presented in Section 5.2.2.2. The second part severely penalized ‘self-coincidence’, and the third part penalized transitions that resulted in an increase in excitation energy.

5.3.4 Difficulties

While the transition space approach seemed reasonable, a few difficulties were encountered. Firstly, converting from transition space to level space can be difficult, especially for schemes that do not obey energy conservation. Secondly, the lack of complex mutations increased the likelihood of only locating a local minima.

It is likely that using a ‘coincidence present/not present’ approach, as used in the level space representation, would significantly improve this approach for two reasons. Firstly, it reduces the solution space. Secondly, using a binary approach it could be easier to examine two transitions and determine if they shared an origin or a destination. (Common entries in rows/columns of the adjacency matrix would indicate shared destination/source levels.) This approach may facilitate the development of complex mutations without requiring further development of transition space to level space conversion algorithms. Instead, methods discussed in 2.2.2.3 could be used. In the non-binary cases, these methods will often give ambiguous results, as many transition space candidate solutions have non-physical aspects (most frequently resulting from transitions decaying to multiple levels). In the binary situation, it would be easier to force transitions to decay to a single level, as branching ratios can be ignored.

5.3.4.1 Doublets

This representation was not tested with doublets as it is insufficiently powerful to be useful in its current form. There are two possible methods of approaching doublets in this representation. Firstly, doublets could be approached in the same fashion as for the level space representation. This would be implemented by having two rows/columns of the adjacency matrix correspond to the same energy of transition, with the expected coincidences from the two transitions being summed before their comparison to the experimental coincidence matrix.

The second approach takes advantage of the doublet signature in transition space, and has one row/column correspond to the doublet, with the doublet being identified after convergence. This approach removes the problem of predetermining doublets. Unfortunately, as the doublet transition should now be placed in two locations in the level scheme, it would play havoc on energy conservation, as well as increasing the difficulty of developing complex mutations.

5.3.5 Results

The transition space representation worked well for schemes with 10 transitions and 6 levels, with calculations performed on the order of minutes. Implementing ideas incorporated into the level space representation, as presented in Section 5.2 to this representation would enable the use of this method for larger level schemes. However, the primary limitation of this representation is the lack of complicated mutation operators - the development of which would require a substantial improvement in automated transition space to level space conversion algorithms.

5.4 Energy ordering of transitions in transition space

5.4.1 Introduction

Given a directed coincidence matrix, it is possible to directly calculate the adjacency matrix using Equation (3.6). Therefore, one approach to level scheme determination is to devise a method of determining the directed coincidence matrix.

Under the assumption that there are no doublets in the coincidence matrix, it is possible to determine the directed coincidence matrix from the energy ordering of the source (or destination) levels of the transitions. Using the directed coincidence matrix and the singles matrix, it is possible to calculate the adjacency matrix, and hence the level scheme, from Equation (3.6). As a result, the energy ordering of the transitions

can be used as a representation. Using this representation gives $n!$ possible solutions - far fewer than the number of possible solutions in the other methods.

This approach determined level schemes with 150 transitions and 60 levels in hours. Furthermore, this representation did not require the use of hill climbing algorithms, complicated mutations or other supplementary algorithms. As a result, this representation is sufficiently flexible to adapt to experimental data.

5.4.2 Methodology

5.4.2.1 Mutations

In this representation two classes of mutations were used. The first class consists of moving one transition, or a group of contiguous transitions to another location in the energy ordering. The second class consists of flipping the ordering of a group of contiguous transitions.

5.4.3 Selection and Replacement

For this representation, the method of selecting candidate solutions for reproduction was modified from the method shown in figure 2.15. In each iteration, the candidate solutions were grouped into groups of four. The two least-fit solutions were replaced by solutions created by applying a crossover operator on one of the most fit solutions and one of the least fit solutions, with the output replacing the least fit solution - as shown in Figure 5.5. This modification was performed in an attempt to increase population diversity and to accommodate the crossover operator presented in section 5.4.3.1.

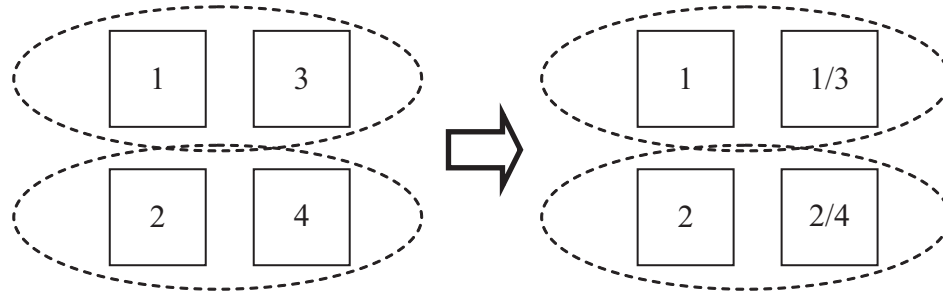


Figure 5.5: For the transition ordering representation, the evolutionary algorithm was modified to apply the crossover operator to act on one of the best two candidate solutions and one of the worst two candidate solutions, with the new solution replacing the worse solution.

5.4.3.1 Crossover

The crossover operator used consisted of first calculating a random weighting for each solution. The weighted ‘average position’ of each transition was then calculated, by multiplying the solution weighting by the position numbering. Transitions in the new candidate solution were then ordered by the ‘average position’.

5.4.3.2 Fitness Testing

Since the adjacency matrix is calculated from a directed coincidence matrix, there is perfect agreement between the expected and experimental coincidence matrices, and as a result fitness checks cannot be based on differences between the coincidence matrices. Fitness tests must therefore be based on the adjacency matrix, and its physical feasibility

The fitness function consisted of two parts. The first part was calculated by summing the squares of all negative elements in the adjacency matrix. This will, however not work well with doublets, though this problem could be mitigated by only summing the squares of negative elements that are not part of the characteristic ‘cross’ pattern associated with doublets, as per Section 3.5.1.

The second part of the fitness function penalizes schemes for transitions with

a total branching ratio greater than one (excluding negative components). This is accomplished by adding $(total\ branching\ ratio - 1)^2$ to the fitness function.

5.4.3.3 Growing The Level Scheme

Due to the use of transition space and the absence of energy conservation based fitness functions, transitions can be added freely to any part of the scheme with little effect. As a result, it is possible to start with a subset of the transitions in the level scheme, iterate until reaching a minimum, then increase the number of transitions used.

However, best results were obtained when starting with the complete level scheme.

5.4.4 Reordering Transitions based on Calculated Energies

Best results were obtained by reordering the transitions based on the calculated transition starting energies. The energies were calculated with a greedy algorithm, similar to the algorithm used for level space schemes, presented in Section 5.2.2.1. However, this method fails when combined with growing the level scheme, as the variable energy associated with vertices that represent more than one transition cannot be automatically taken into account, which results in transitions being reordered into the incorrect energy ordering location.

5.4.5 Difficulties

The two largest difficulties faced by this method are the size of solution space and the presence of doublets. The solution space has $n!$ possible solutions, where n is the number of transitions. While the solution size is far smaller than the solution spaces for the other representations, factorially growing solutions sizes still pose a significant challenge.

The presence of doublets violates the assumptions of this representation. In general, it is impossible to assign a specific place in the energy ordering to the doublet, as

each transition in the doublet should be placed independently. This creates problems when the two transitions in the doublet are in related parts of the level scheme. This difficulty can be overcome through the use of tricks. In particular, since transitions can be added to the level scheme in any order without disturbing the structure of the level scheme, it would be possible to construct the scheme excluding doublet transitions, and manually add the doublets at the end. Unfortunately, this method requires prior knowledge regarding which transitions are doublets. It would be possible to iteratively attempt to use this method to solve a level scheme, then identify and remove transitions that exhibit characteristics of doublets - as discussed in Section 3.5.1 - until a ‘correct’, doublet-free level scheme was found. The doublet transitions could then be reintroduced into the level scheme.

5.4.6 Results

This representation was the most successful of the three examined, and facilitated the solution of doublet-free level schemes with up to approximately 150 transitions and 60 levels in the presence of Poisson distributed errors. These results were obtained starting from a full set of transitions and reordering transitions based on their calculated energies. Calculations took on the order of hours on a laptop.

It is probable that using faster computers for longer periods of time with larger numbers of candidate solutions would enable the calculation of larger level schemes.

5.4.7 Future Work

While most level schemes of interest contain more than 150 transitions, it should be possible to take a large data set (consisting of perhaps of 300 transitions), and break it into a number of smaller overlapping data sets, with each of the smaller data sets containing around 150 transitions - which could then be solved. The solutions from the smaller data sets could then be used to reconstruct the larger scheme, as most

regions of the full level scheme would be reproduced in one or more of the smaller solutions.

One possible method for breaking the large data set into smaller data sets would be using the following algorithm:

1. Create a new data set consisting of n clustered transitions in the data set (the ‘seed’). Varying n will determine the size of the smaller data sets - each of the smaller data sets should be large, though easy to compute (Perhaps including 100 transitions).
2. Add all transitions that are in coincidence with the original n transitions to the data set.
3. Solve the smaller data set.
4. Repeat this process until all transitions have been one of the original n transitions in a data set.

Using this method, the data set ‘seeded’ with any given transition would likely include the correct structure around that transition.

Chapter 6

Conclusion and Future Work

Results presented in this work strongly suggest that automated nuclear level scheme determination is feasible, though there are still substantial challenges. This work primarily consisted of the development of a new approach to calculating nuclear levels schemes, and the investigation of various computer-automated methods of accomplishing this task.

The use of transition space, and the associated analytical formula provides a direct method of constructing level schemes based on their connectivity. Transition space provides a representation where transitions and the relationships between them can be explored abstractly, without requiring the assignment of source and destination levels. This representation combines favourably with γ -ray spectroscopy experiments, as these experiments measure γ rays and the relationships between them - they do not directly measure any energy level information. Furthermore, the use of transition space enables the application of the analytical formula derived in Section 3.3, which directly relates a transition space level scheme to the singles and the directed coincidence data. However, the power and flexibility accorded by the use of transition space and the analytical formula comes at a price - it is non-trivial to convert transition space level schemes to level space. There are also challenges in determining the

directed coincidence data - since γ -ray spectroscopy experiments can only measure undirected coincidence data.

A number of automated methods of level scheme construction were investigated. These consisted of a self-consistent variation of the analytical formula that used non-directed coincidence data as well as a number of different evolutionary algorithm based approaches.

The evolutionary algorithm approaches differed by the representation used for the level schemes. Three representations were used: a level space representation, a transition space representation, and a transition ordering representation. The transition ordering representation was by far the most successful representation - capable of solving simulated doublet-free level schemes with up to 150 transitions and 60 levels, in the presence of Poisson distributed errors.

The transition ordering representation demonstrates the possibilities of automated nuclear level scheme determination. However, there are still a substantial number of challenges to overcome. The most significant obstacle is the shift from simulated data to experimental data - and all the myriad complications thus introduced. Experimental data introduces challenges resulting from non-zero experimental backgrounds, huge order of magnitude differences in intensity, many doublets and complications arising from physical level schemes. It will be interesting to observe how the effects of these different complications interact, and how they can be resolved - especially since it would be extremely difficult to accurately model their interactions, or to overcome the obstacles without an accurate picture of how they interact.

Furthermore, methods of quickly and accurately constructing reduced singles matrices and reduced coincidence matrices must be developed for automated nuclear level scheme determination to be useful - as it takes months to accurately calculate the intensities of all coincidences in a data set. This is especially true since the calculation of the intensities is performed concurrently with the construction of a level

scheme, and as a result an automated method would not be useful. However, work required for the automatic construction of the reduced matrices is underway [10]. Alternatively, it would be relatively straightforward to create a software package that displayed and fit two-dimensional peaks, allowing a user to quickly and easily vary fit parameters to compensate for various backgrounds, ridges and doublets, which is difficult to accomplish automatically.

While there is still a significant amount of work before automated nuclear level scheme determination becomes a reality, it appears that the remaining challenges are surmountable, and that automated nuclear level scheme determination will become incredibly useful - especially with the ongoing development of increasingly powerful γ -ray spectrometers.

Appendix A

Representations of Level Space

Schemes in Transition Space

This appendix contains the building blocks required to schematically convert level space schemes to transition space schemes.

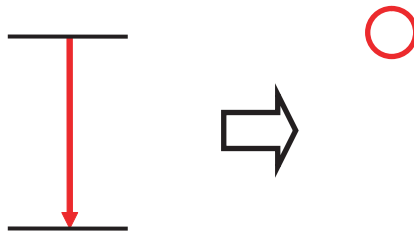


Figure A.1: Single transitions are represented as isolated vertices in transition space.

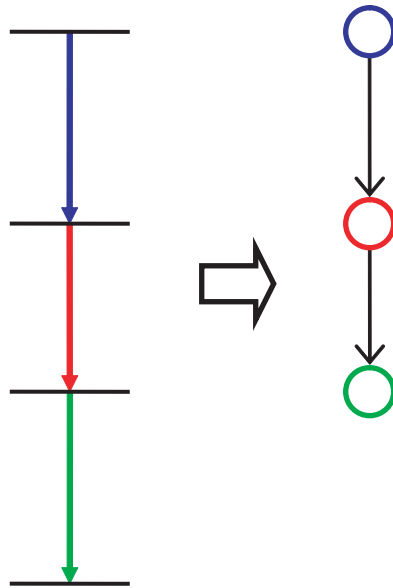


Figure A.2: Chains of transitions are represented as chains of vertices.

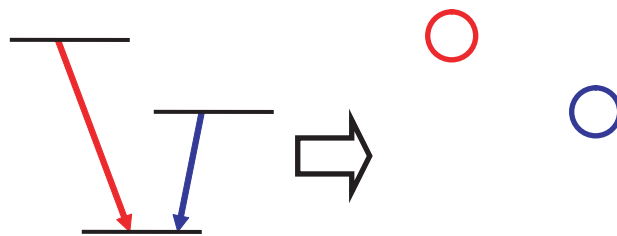


Figure A.3: There is no connectivity between two transitions decaying to a level.

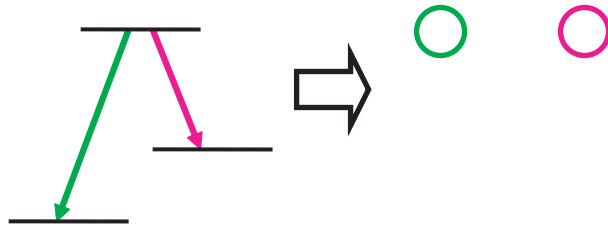


Figure A.4: There is also no connectivity between two transitions decaying from a level.

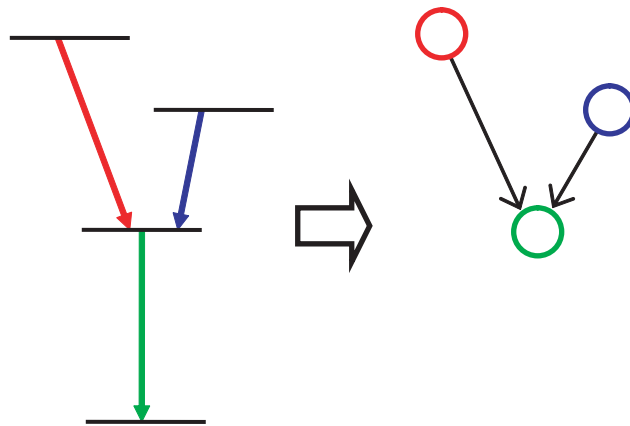


Figure A.5: There is an edge from each of the incoming transitions to the transition decaying from the level.

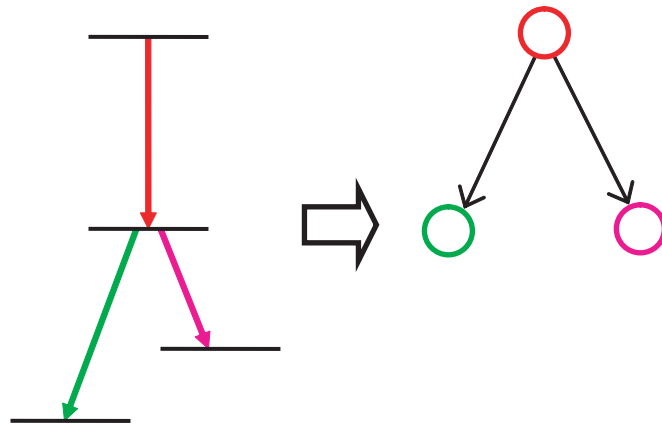


Figure A.6: There is an edge from the incoming transition to both of the outgoing transitions.

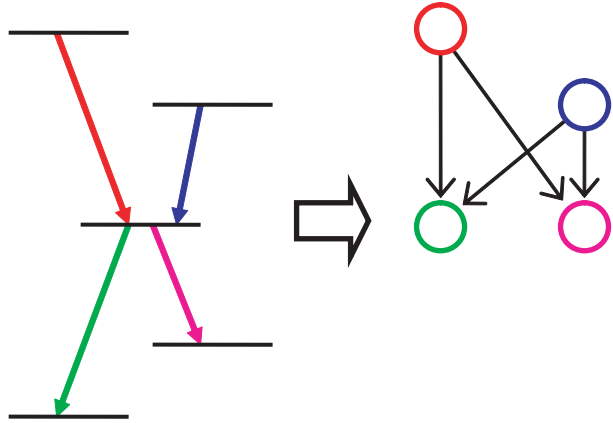


Figure A.7: Edges are placed from all incoming transitions to all outgoing transitions.

Appendix B

Converting from Transition Space to Level Space

B.1 Introduction

Transition space is useful for level scheme determination as it closely parallels the structure of the experimental data and emphasizes the connectivity of level schemes. As a result, it is an excellent tool for level scheme determination. However, level space schemes are easier to interpret, and therefore transition space schemes should be converted to level space after determination. In this appendix, some characteristics of level space level schemes produced from transition space level schemes are discussed, and an algorithm with an example for converting transition space schemes to level space schemes is presented.

B.2 Characteristics of Level Schemes Converted From Transition Space

Nuclear γ -ray spectroscopy experiments detect γ rays emitted when a nucleus decays from one level to another. As a result, the data obtained relates to transitions, and relationships between transitions. The data does not directly relate to energy levels. Therefore, if two transitions decay from the same energy, it is impossible to determine the number of energy levels at that energy, unless a third transition decays into one or both of the two transitions. As a result, level space schemes created from transition space schemes show two energy levels at the same energy to highlight the undetermined nature of the level for the experimenter. A similar effect occurs for the case of two transitions decaying into a level from which no transitions decay. An example of a level space scheme produced from a transition space scheme is presented in Figure B.1.

B.3 Transition Space to Level Space Algorithm

Transition space schemes can be converted to level space through the following algorithm:

- Multiply the singles matrix and the adjacency matrix to create a weighted adjacency matrix.
- While there exist transitions that have not been placed:
 - Place the transitions associated with the largest overall weighted adjacency matrix value. If no transitions have a positive adjacency matrix value, place the transition associated with the largest singles matrix value.
 - While there are transitions adjacent to already placed transitions:

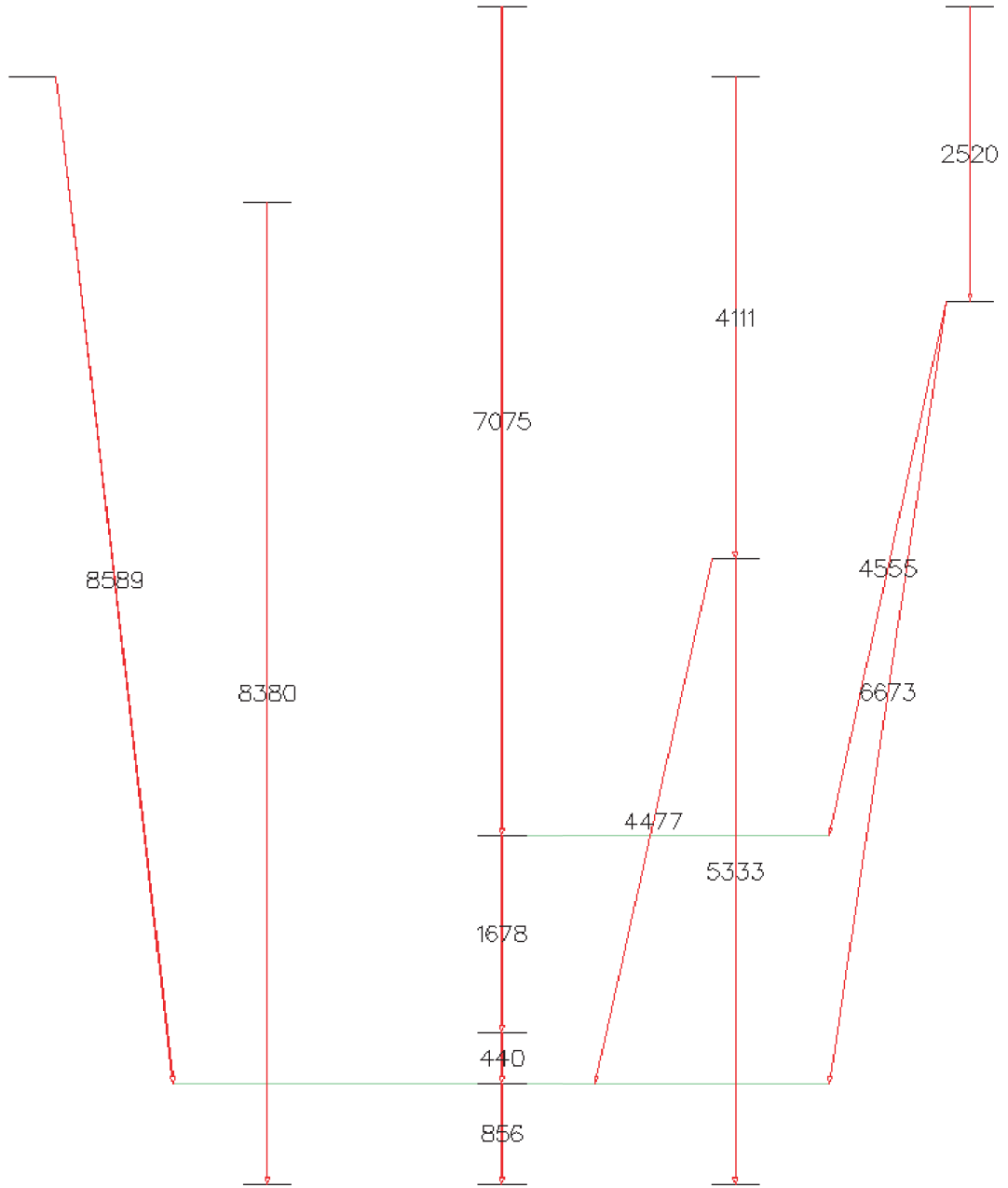


Figure B.1: A level space scheme created from a transition space scheme.

- * Add the adjacent transition with the largest weighted adjacency value connected to an already placed transition.
- Examine levels with similar energies, and determine if they are level doublets.
- Resolve contradictions in level energies caused by unobserved transitions and doublets. Determine if new level doublets have been introduced.
- Shift the ground state energy to zero.

B.4 An Example of Converting from Transition Space to Level Space

Given a transition space adjacency matrix as shown in Figure B.2 and a singles matrix as shown in Figure B.3, a weighted adjacency matrix can be calculated, as shown in Figure B.4, as per appendix B.3.

$$Adjacency = \begin{pmatrix} & 2507 & 2540 & 4117 & 4150 & 4187 & 4945 & 5797 & 8337 & 9094 & 13282 \\ \hline 2507 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 2540 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 4117 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 4150 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 4187 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 4945 & 0 & 0.70 & 0 & 0.23 & 0 & 0 & 0 & 0.07 & 0 & 0 \\ 5797 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 8337 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 9094 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 13282 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

Figure B.2: A transition space adjacency matrix.

As the greatest weighted adjacency value is between the 2540 keV transition and the 5797 keV transition place these transitions in the level scheme.

$$\begin{array}{l}
\text{Singles} = \left(\begin{array}{c|ccccccccccc}
& 2507 & 2540 & 4117 & 4150 & 4187 & 4945 & 5797 & 8337 & 9094 & 13282 \\
\hline
2507 & 228 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
2540 & 0 & 1767 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
4117 & 0 & 0 & 546 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
4150 & 0 & 0 & 0 & 565 & 0 & 0 & 0 & 0 & 0 & 0 \\
4187 & 0 & 0 & 0 & 0 & 2629 & 0 & 0 & 0 & 0 & 0 \\
4945 & 0 & 0 & 0 & 0 & 0 & 191 & 0 & 0 & 0 & 0 \\
5797 & 0 & 0 & 0 & 0 & 0 & 0 & 6491 & 0 & 0 & 0 \\
8337 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 179 & 0 & 0 \\
9094 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 298 & 0 \\
13282 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 698
\end{array} \right)
\end{array}$$

Figure B.3: A singles intensity matrix.

$$\begin{array}{l}
\text{Weighted Adjacency} = \left(\begin{array}{c|ccccccccccc}
& 2507 & 2540 & 4117 & 4150 & 4187 & 4945 & 5797 & 8337 & 9094 & 13282 \\
\hline
2507 & 0 & 0 & 0 & 0 & 0 & 0 & 228 & 0 & 0 & 0 \\
2540 & 0 & 0 & 0 & 0 & 0 & 0 & 1767 & 0 & 0 & 0 \\
4117 & 0 & 0 & 0 & 0 & 546 & 0 & 0 & 0 & 0 & 0 \\
4150 & 0 & 0 & 0 & 0 & 565 & 0 & 0 & 0 & 0 & 0 \\
4187 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
4945 & 0 & 134 & 0 & 43 & 0 & 0 & 0 & 14 & 0 & 0 \\
5797 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
8337 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
9094 & 0 & 0 & 0 & 0 & 298 & 0 & 0 & 0 & 0 & 0 \\
13282 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{array} \right)
\end{array}$$

Figure B.4: A weighted adjacency matrix calculated from the singles matrix and the adjacency matrix.

Sequentially adding the most intense adjacent transitions, the 2507, 4945, 4150, 4187, 4117, 9094 and 8337 keV transitions are added.

As all transitions connected to the 2540 keV transition have been placed, place the only remaining transition - the 13282 keV transition.

After all transitions have been placed, examine levels with similar energies and determine if the levels are doublet levels. For this example, the levels at 8304 and 8337 keV are at similar energies. However, upon examination of the weighted adjacency matrix it is clear that there are at least two levels (and it is possible that there is a level doublet at 8304 keV).

Finally, shift the energies such that the 4187, 5797, 8337, and 13282 keV transitions decay to the ground state at 0 keV.

The produced level scheme is presented in Figure B.5.

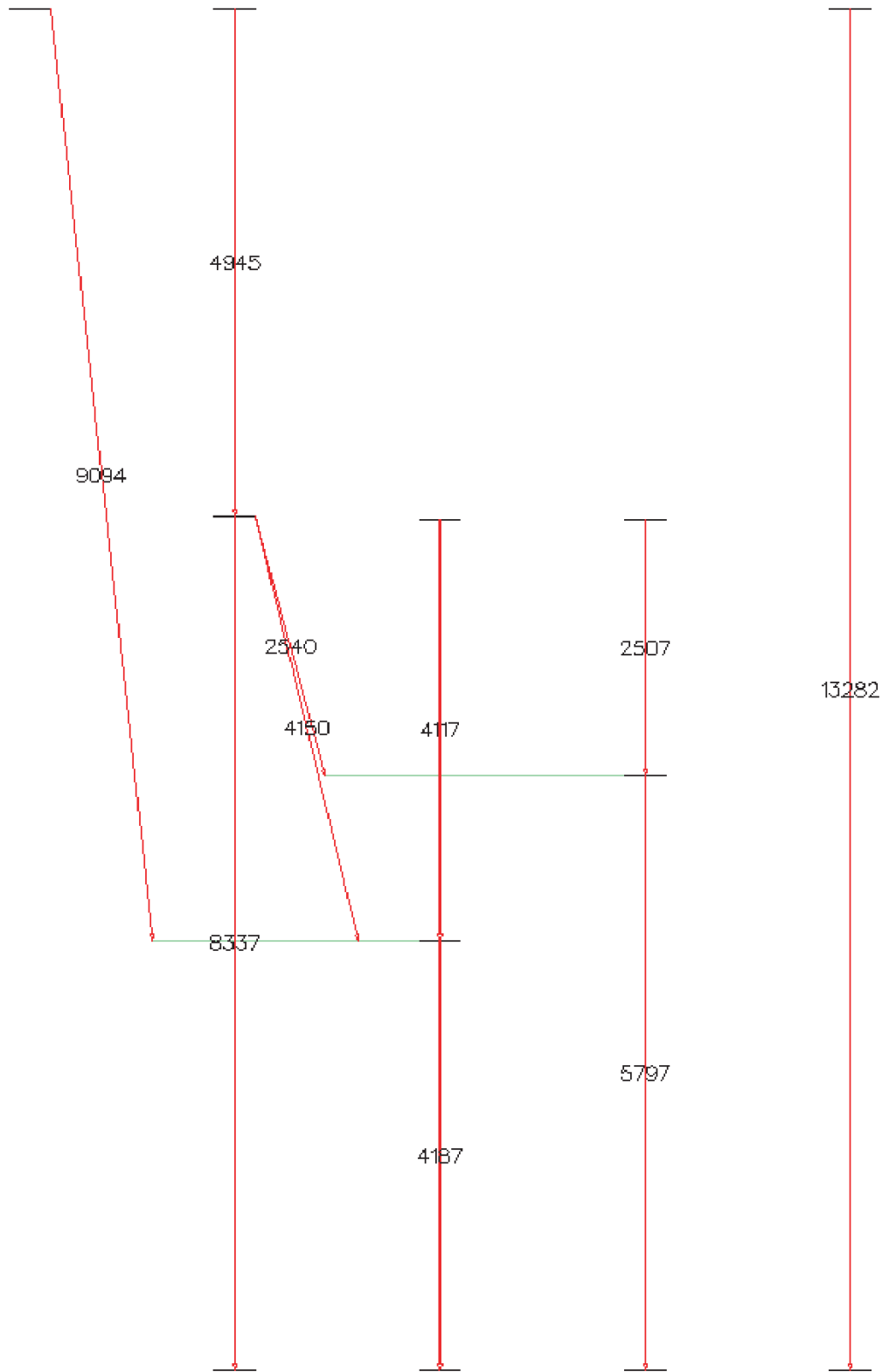


Figure B.5: The level space scheme produced from the adjacency matrix in Figure B.2 and the singles matrix in Figure B.3.

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