Solutions to Systems of Differential Equations having Degenerate Eigenvalue Structure

C. Sean Bohun[1)] and Mark S. Welsh[2)]

[1)] *Department of Mathematics and Physics, University of Victoria, P. O. Box 3045, Victoria, British Columbia, Canada V8W 3P4*
[2)] *Department of Physics and Astronomy, University of Victoria, P. O. Box 3055, Victoria, British Columbia, Canada V8W 3P6*

(TRIUMF preprint TRI-PP-93-7)

A method of solution has been developed for systems of linear, first order, ordinary differential equations (ODEs) having a degenerate eigenvalue structure. This method takes advantage of the degeneracy to determine the possible form which the solution may take. The basis functions of which the solution is constructed are found by consideration of the Jordan canonical form of the ODEs' rate matrix. The specific solution is then computed by substitution of this form into the original ODEs, giving rise to a series of recurrence relationships. These are solved explicitly for a particular example, thus demonstrating the techniques necessary for the solution of an arbitrary set of ODEs possessing this degenerate structure. The importance of this work lies in the case where the number of coupled ODEs is allowed to increase, while the degenerate structure is preserved. The difficulty of solution increases only slightly with such an increase in the dimension of the problem. This is in stark contrast to the traditional method of solution, where the construction of a diagonalizing matrix becomes substantially less tractible with increasing dimension.
PACS Numbers 02.10.S, 02.30.H

1 Introduction

In many areas of physics there arise systems of coupled, linear, ODE's with a large number of degenerate eigenvalues. A couple of examples of these types of systems are radioactive decay chains, and pumping of nuclear spin states. For the problems that we are considering, one can construct a vector

$$\mathcal{P}(t) = \langle P_1(t), P_2(t), P_3(t), \ldots \rangle$$

where each $P_j(t)$ represents the population of the state j as a function of time. In this case, the system can then be written as

$$\frac{d}{dt}\mathcal{P}(t) = A\mathcal{P}(t) \tag{1}$$

where A is some time-independent, complex valued, square matrix constructed through consideration of the physical rates linking the populations.

In this article we present a method of solution, appropriate when there is a repetitive structure in A leading to a degeneracy in its eigenvalues. The method is of particular value when solving for a set of populations where the rate matrix A is of arbitrary dimension, and where the number of independent eigenvalues remains the same as the matrix dimension is changed. In order to clarify the techniques used in this paper we shall employ a particular form for the matrix A, namely,

$$A = \begin{pmatrix}
-\beta & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 \\
\beta & -\alpha & \alpha & 0 & 0 & & & 0 & 0 & 0 \\
0 & \alpha & -\alpha-\beta & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 \\
0 & 0 & \beta & -\alpha & \alpha & & & 0 & 0 & 0 \\
0 & 0 & 0 & \alpha & -\alpha-\beta & \cdots & \cdots & 0 & 0 & 0 \\
\vdots & & \vdots & & \vdots & \ddots & & \vdots & & \vdots \\
\vdots & & \vdots & & \vdots & & \ddots & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \cdots & \beta & -\alpha & \alpha & 0 \\
0 & 0 & 0 & 0 & 0 & & 0 & \alpha & -\alpha-\beta & 0 \\
0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & \beta & 0
\end{pmatrix}. \tag{2}$$

Notice that where there are N repetitions of the block

$$\begin{pmatrix} \beta & -\alpha & \alpha \\ 0 & \alpha & -\alpha-\beta \end{pmatrix}$$

and the dimension of A is $2N+2$.

In Section 2 we shall consider a reduction to Jordan canonical form of the matrix A. This proves not to be a tractable procedure for rate matrices of arbitrary dimension, but does give rise to a set of basis functions for the solution. These functions are used in Section 3 where we present our method of solution by substitution. Section 3 is a detailed calculation dealing mainly with our example matrix (2), but the method may be applied to other rate matrices with a similar degenerate eigenvalue structure.

Finally, in Section 4, a solution is fully developed for the example rate matrix using certain approximations involving the rates α and β. A comparison is then made to a similar problem which arises in the context of spin pumping and relaxation in nuclear physics.

2 Solution by Jordan Form

The existence of a unique solution to a matrix equation of the form

$$B\frac{d}{dt}\mathcal{P}(t) = A\mathcal{P}(t),$$

where A and B are square complex valued matrices, is guaranteed provided there exists a $\lambda \in \mathbb{C}$ such that $(A-\lambda B)^{-1}$ exists [1]. For the special case where $B = I$ this reduces to finding a λ that is *not* an eigenvalue of A. Clearly, for a finite dimensional matrix such as ours, a unique solution always exists.

One might naïvely attempt to find a solution of the system by noting that

$$\mathcal{P}(t) = e^{At}\mathcal{P}(0).$$

We can now write $A = CJC^{-1}$, where C is a non-singular matrix constructed such that J is in Jordan canonical form. We then note that

$$e^{At} = Ce^{Jt}C^{-1}.$$

This is trivially seen by expansion of the matrix exponentials.

To discern the Jordan matrix J and the diagonalizing matrix C we must first find the eigenvalues of A. For the example rate matrix given in (2), these eigenvalues λ are given by $\det[A-\lambda I] = 0$ which implies that

$$\lambda(\lambda+\beta)(\lambda^2 + (2\alpha+\beta)\lambda + \alpha\beta)^N = 0.$$

Thus our eigenvalues are 0 and $-\beta$ with degeneracy of one, and

$$\lambda_{\pm} = -\alpha - \frac{\beta}{2} \pm \Delta; \qquad \Delta^2 = \alpha^2 + \frac{\beta}{4}^2$$

each with degeneracy N.

The most general Jordan form of A, assuming $\dim(\{\mathbf{v} \mid A\mathbf{v} = \lambda\mathbf{v}\}) = 1$ for each of $\lambda = \lambda_{\pm}$, is therefore

$$Jt = \begin{pmatrix} 0 & & & \\ & -\beta t & & \\ & & [Jt]_+ & \\ & & & [Jt]_- \end{pmatrix},$$

where we define the $N \times N$ matrices

$$[Jt]_{\pm} = \begin{pmatrix} \lambda_{\pm}t & 1 & & & \\ & \lambda_{\pm}t & 1 & & \\ & & \ddots & \ddots & \\ & & & \ddots & 1 \\ & & & & \lambda_{\pm}t \end{pmatrix}.$$

It can be shown [2] that

$$e^{Jt} = \begin{pmatrix} 1 & & & \\ & e^{-\beta t} & & \\ & & B_+ & \\ & & & B_- \end{pmatrix}; \qquad B_\pm = e^{\lambda_\pm t} \begin{pmatrix} 1 & \frac{(\lambda_\pm t)}{1!} & \frac{(\lambda_\pm t)^2}{2!} & \cdots & \frac{(\lambda_\pm t)^{N-1}}{(N-1)!} \\ & 1 & \frac{(\lambda_\pm t)}{1!} & \cdots & \frac{(\lambda_\pm t)^{N-2}}{(N-2)!} \\ & & \ddots & \ddots & \vdots \\ & & & \ddots & \frac{(\lambda_\pm t)}{1!} \\ & & & & 1 \end{pmatrix}.$$

The Jordan canonical form for A generates a set of basis functions on which to construct a solution. In this case these are,

$$\{1, e^{-\beta t}, t^n e^{\lambda_+ t}, t^n e^{\lambda_- t}\}; \qquad n = 0, 1, \ldots, (N-1). \tag{3}$$

The span of this set of functions is guaranteed to form a basis for solutions to (1) provided $\Delta \neq 0$. However, depending on the exact Jordan canonical form, certain functions may not be required.

The next step in the procedure would be to compute the eigenvectors of A, form the matrix C and its inverse, and to then compute $Ce^{Jt}C^{-1}$. Clearly we shall encounter substantial problems during this calculation.

Due to the degeneracy of the eigenvalues $\lambda_\pm$, we may not be able to find N independent eigenvectors of A. The remaining columns of C are formed with generalized eigenvectors of A. This involves finding the 1^{st} to, at worst, the $(N-1)^{st}$ generalized eigenvectors by solving

$$(A - \lambda_\pm I)^j \mathbf{v}_{\pm j} = 0,$$

where

$$(A - \lambda_\pm I)^{j-1} \mathbf{v}_{\pm j} \neq 0; \qquad j = 2, 3, \ldots N.$$

This is found to be an arduous task even for the 1^{st} generalized eigenvectors of $\lambda_\pm$.

Supposing that C could be constructed, one would then have to find C^{-1} and finally $Ce^{Jt}C^{-1}$. The inversion of a $2N+2$ dimensional matrix is certainly not trivial. The correct expression for the Jordan canonical form is also not immediately clear, and it is this expression which dictates the number of generalized eigenvectors which must be found.

It is apparent that a calculation of the $P_j(t)$ would be extremely difficult for all but the lowest values of N. There is, however, another possible method of solution which will be outlined in the following section.

3 Solution by Substitution

We now proceed to solve the particular example rate matrix (2). While the reformulation presented in Section 3.1 would be of the same form for a general matrix A with repetitive eigenvalue structure, the solution in Section 3.2 is quite specific to our particular example.

3.1 Reformulation of the Problem

We have noted that the time dependence of the $P_j(t)$ may be constructed from a limited number of known basis functions, given in (3). The solutions may be written as

$$P_j(t) = a_{j,1} + a_{j,2}e^{-\beta t} + \sum_{n=0}^{N-1} t^n (b_{j,n}e^{\lambda_+ t} + w_{j,n}e^{\lambda_- t}); \qquad j = 1, \ldots, 2N+2. \tag{4}$$

This implies

$$\begin{aligned} \frac{d}{dt}P_j(t) &= -\beta a_{j,2}e^{-\beta t} \\ &\quad + \sum_{n=0}^{N-2} t^n \left\{[\lambda_+ b_{j,n} + (n+1)b_{j,n+1}]e^{\lambda_+ t} + [\lambda_- w_{j,n} + (n+1)w_{j,n+1}]e^{\lambda_- t}\right\} \\ &\quad + t^{N-1}(\lambda_+ b_{j,N-1}e^{\lambda_+ t} + \lambda_- w_{j,N-1}e^{\lambda_- t}). \end{aligned} \tag{5}$$

Substituting (4) and (5) into (1) with rate matrix (2) yields the system of differential equations

$$\begin{array}{lllll} P_1' & & +\beta P_1 & & =0 \\ P_{2l}' & -\beta P_{2l-1} & +\alpha P_{2l} & -\alpha P_{2l+1} & =0 \\ P_{2l+1}' & & -\alpha P_{2l} & +(\alpha+\beta) P_{2l+1} & =0 \\ P_{2N+2}' & -\beta P_{2N+1} & & & =0 \end{array} \tag{6}$$

where the prime denotes differentiation with respect to time and $l = 1, 2, \ldots, N$. The linear independence of our basis functions allows us to combine (4), (5) and (6) and to equate the coefficients of each member of the basis. This gives a system of relations between the constants $a_{j,1}$, $a_{j,2}$, $b_{j,n}$ and $w_{j,n}$ ($j = 1, 2, \ldots, 2N+2$; $n = 0, 1, \ldots, N-1$). We also have the $2N + 2$ initial conditions

$$P_j(0) = a_{j,1} + a_{j,2} + b_{j,0} + w_{j,0}. \tag{7}$$

The method of solution now shifts from one of finding the appropriate Jordan canonical form for A to one of solving a system of recurrence relationships among the coefficients of the $P_j(t)$. The latter method is more amenable to solution in the case of arbitrary N.

3.2 An Explicit Representation of the Solution

We will now explicitly solve (6) with initial conditions (7). We shall compute the coefficients $a_{j,1}$ and $a_{j,2}$ of the time-dependent populations corresponding to the eigenvalues $\lambda = 0$ and $\lambda = -\beta$. For the coefficients of the degenerate eigenvalues, the $b_{j,n}$ and $w_{j,n}$, we proceed in three steps. First, we discover which coefficients are found to be identically zero. Then we obtain and solve sets of recurrence relations for the remaining coefficients $b_{j,n}$ and $w_{j,n}$, in terms of the $b_{j,0}$ and $w_{j,0}$. Finally, one determines the $b_{j,0}$ and $w_{j,0}$ from the initial data, $P_j(0)$.

Collecting the relations for the $a_{j,1}$ one obtains

$$\begin{aligned} \beta a_{1,1} &= 0 && \text{(8.a)} \\ -\beta a_{2l-1,1} + \alpha a_{2l,1} - \alpha a_{2l+1,1} &= 0 && \text{(8.b)} \\ -\alpha a_{2l,1} + (\alpha+\beta) a_{2l+1,1} &= 0 && \text{(8.c)} \\ -\beta a_{2N+1,1} &= 0 && \text{(8.d)} \end{aligned}$$

where $l = 1, 2, \ldots, N$. Adding (8.b) and (8.c) we obtain $a_{2l+1,1} = a_{2l-1,1}$ which, by virtue of the boundary conditions (8.a) and (8.d), imply that $a_{j,1} = 0$ when j is odd. Using (8.c), we conclude that $a_{j,1} = 0$ for all j except $j = 2N + 2$.

The $a_{j,2}$ yield the following relationships:

$$\begin{aligned} -\beta a_{2l-1,2} + (\alpha-\beta) a_{2l,2} - \alpha a_{2l+1,2} &= 0 && \text{(9.a)} \\ -\alpha a_{2l,2} + \alpha a_{2l+1,2} &= 0 && \text{(9.b)} \\ -\beta a_{2N+1,2} - \beta a_{2N+2,2} &= 0. && \text{(9.c)} \end{aligned}$$

Adding (9.a) and (9.b) gives $a_{2l,2} = a_{2l+1,2} = -a_{2l-1,2}$. Therefore $a_{2l,2} = a_{2l+1,2} = (-1)^l a_{1,2}$ which holds for $l = 1, 2, \ldots, N$ with $a_{2N+2,2} = (-1)^{N+1} a_{1,2}$. We can now give the $a_{j,1}$ and $a_{j,2}$ in terms of the initial conditions by noting two distinct relationships. First,

$$P_1(t) = P_1(0) e^{-\beta t},$$

which implies that $a_{1,2} = P_1(0)$. Secondly, since the sum down each column of the rate matrix (2) is zero, $\sum_{j=1}^{2N+2} P_j'(t) = 0$. Therefore,

$$\sum_{j=1}^{2N+2} P_j(t) = \text{constant} = \sum_{j=1}^{2N+2} P_j(0)$$

which must be $a_{2N+2,1}$. Hence,

$$a_{k,1} = \begin{cases} \sum_{j=1}^{2N+2} P_j(0); & k = 2N+2 \\ 0; & \text{otherwise} \end{cases} \tag{9.d}$$

and

$$\begin{aligned} a_{1,2} &= P_1(0) && \text{(9.e)} \\ a_{2k,2} = a_{2k+1,2} &= (-1)^k P_1(0); \quad k = 1, 2, \ldots, N && \text{(9.f)} \\ a_{2N+2,2} &= (-1)^{N+1} P_1(0). && \text{(9.g)} \end{aligned}$$

The relations for the $b_{j,n}$, or equivalently for the $w_{j,n}$, are more complicated. Indeed, their solution shall be the concern of the remainder of this section. The relations are given by

$$\begin{aligned} (\beta + \lambda_+) b_{1,n} + (n+1) b_{1,n+1} &= 0 && \text{(10.a)} \\ (\beta + \lambda_+) b_{1,N-1} &= 0 && \text{(10.b)} \\ -\beta b_{2l-1,n} + (\alpha + \lambda_+) b_{2l,n} + (n+1) b_{2l,n+1} - \alpha b_{2l+1,n} &= 0 && \text{(10.c)} \\ -\beta b_{2l-1,N-1} + (\alpha + \lambda_+) b_{2l,N-1} - \alpha b_{2l+1,N-1} &= 0 && \text{(10.d)} \\ -\alpha b_{2l,n} + (n+1) b_{2l+1,n+1} + (\alpha + \beta + \lambda_+) b_{2l+1,n} &= 0 && \text{(10.e)} \\ -\alpha b_{2l,N-1} + (\alpha + \beta + \lambda_+) b_{2l+1,N-1} &= 0 && \text{(10.f)} \\ -\beta b_{2N+1,n} + \lambda_+ b_{2N+2,n} + (n+1) b_{2N+2,n+1} &= 0 && \text{(10.g)} \\ -\beta b_{2N+1,N-1} + \lambda_+ b_{2N+2,N-1} &= 0 && \text{(10.h)} \end{aligned}$$

where $l = 1, 2, \ldots, N$ and $n = 0, 1, \ldots, N-1$. The corresponding relations amongst the $w_{j,n}$ can be obtained with the substitutions $b_{j,n} \to w_{j,n}$ and $\lambda_+ \to \lambda_-$. Because of this correspondence, we will focus on the $b_{j,n}$.

There are a number of the $b_{j,n}$ which can be shown to be zero in general. From (10.b) we have $b_{1,N-1} = 0$ since in general $\lambda_+ + \beta \neq 0$. Also (10.a) gives $(n+1) b_{1,n} = -(\lambda_+ + \beta) b_{1,n+1}$ which, by induction, gives a recurrence relation implying

$$b_{1,n} = 0; \quad \text{for} \quad n = 0, 1, \ldots, N-1. \tag{11}$$

As well, taking the linear combination α(10.d) + $(\lambda_+ + \alpha)$(10.f), one obtains $-\alpha\beta b_{2l-1,N-1} = 0$ so that $b_{2l-1,N-1} = 0$, where $l = 1, 2, \ldots, N$. Using (10.f), we conclude that

$$b_{j,N-1} = 0 \quad \text{where} \quad j = 1, 2, \ldots, 2N-1 \tag{12}$$

whilst $b_{2N,N-1}$, $b_{2N+1,N-1}$ and $b_{2N+2,N-1}$ are related by

$$b_{2N,N-1} = \frac{\alpha + \beta + \lambda_+}{\alpha} b_{2N+1,N-1} \quad \text{and} \quad b_{2N+1,N-1} = \frac{\lambda_+}{\beta} b_{2N+2,N-1}. \tag{13}$$

This last relation follows from (10.h).

Combining (10.c) and (10.e) we obtain the matrix equation

$$\begin{pmatrix} \alpha & \alpha + \lambda_+ \\ -\alpha & \alpha + \beta + \lambda_+ \end{pmatrix} \begin{pmatrix} b_{2l,n+1} \\ b_{2l+1,n+1} \end{pmatrix} = \begin{pmatrix} \frac{\alpha\beta}{(n+1)} b_{2l-1,n} \\ -(n+2) b_{2l+1,n+2} \end{pmatrix} \tag{14}$$

which is valid for $l = 1, 2, \ldots, N$ and $n = 0, 1, \ldots, N-2$. Notice that

$$\det \begin{pmatrix} \alpha & \alpha + \lambda_+ \\ -\alpha & \alpha + \beta + \lambda_+ \end{pmatrix} = 2\alpha\Delta \neq 0. \tag{15}$$

The procedure for determining which of the remaining $b_{j,n}$ are zero can now be described through a four step process.

Step 1: Set $n = N-3, l = 1$ in expression (14). Using (11) and (12), the right hand side of (14) must be zero. Hence, by (15), we must conclude that $b_{2l,n+1} = b_{2l+1,n+1} = 0$ for these particular values of l and n. Now go to Step 3.

Step 2: From the previous Step 2 the right hand side of (14) must be zero. Hence, by (15), we must conclude that $b_{2l,n+1} = b_{2l+1,n+1} = 0$ for these particular values of l and n. Now go to Step 3.

Step 3: If $n \neq l-1$ then let $n \to n-1$ and return to Step 2, otherwise continue to Step 4.

Step 4: If $l \neq N-2$ then set $n = N-3$, let $l \to l+1$ and return to Step 2, otherwise we are finished.

This procedure reveals that

$$b_{2l,k} = b_{2l+1,k} = 0 \quad \text{for} \quad 1 \le l \le k \le N-1 \tag{16.a}$$

and through an analogous argument

$$w_{2l,k} = w_{2l+1,k} = 0 \quad \text{for} \quad 1 \le l \le k \le N-1. \tag{16.b}$$

The procedure described above is only applicable when $N > 2$. For $N = 1, 2$ those $b_{j,n}$ that are zero are completely described by expressions (11) and (12). The remaining unknown $b_{j,n}$ and $w_{j,n}$ may be solved in terms of the $b_{j,0}$ and $w_{j,0}$ by the derivation of a number of recurrence relations. The $b_{j,0}$ and $w_{j,0}$ may themselves be found in terms of the initial populations $P_j(0)$. The only equations required in the construction of the recurrence relations are (10.c) and (10.e). Specifically, the combination $\alpha(10.c) + (\alpha + \lambda_+)(10.e) + (n+1)(10.e)_{n\to n+1}$, where $n \to n+1$ denotes the substitution of $n+1$ for n in (10.e), yields

$$2\Delta b_{2l+1,n+1} + (n+2) b_{2l+1,n+2} = \frac{\alpha\beta}{(n+1)} b_{2l-1,n}. \tag{17}$$

A similar equation that connects only even elements can be derived by considering the combination $(\alpha + \beta + \lambda_+)(17) + (n+2)(17)_{n\to n+1}$. This simplifies, by using (10.e), to

$$2\Delta b_{2l,n+1} + (n+2) b_{2l,n+2} = \frac{\alpha\beta}{(n+1)} b_{2l-2,n}. \tag{18}$$

At this point we can concentrate on those $b_{j,n}$ with j odd. This can be done without loss of generality since (17) and (18) have the same structure.

Using (16.a) we can conclude that the first nontrivial value of n for (17) is $n = l-2$. For this case, (17) reduces to

$$2\Delta b_{2l+1,l-1} = \frac{\alpha\beta}{(l-1)} b_{2l-1,l-2}.$$

Hence,

$$b_{2l+1,l-1} = \left(\frac{\alpha\beta}{2\Delta}\right)^{l-1} \frac{b_{3,0}}{(l-1)!}. \tag{19}$$

The case $n = l-3$ yields

$$b_{2l+1,l-2} = \frac{\alpha\beta}{2\Delta(l-2)} b_{2l-1,l-3} - \frac{(l-1)}{2\Delta}\left(\frac{\alpha\beta}{2\Delta}\right)^{l-1} \frac{b_{3,0}}{(l-1)!},$$

where we have used (19). This is of the form

$$b_k = \frac{\theta}{k} b_{k-1} + f(k),$$

whose solution is

$$b_k = \frac{\theta^k}{k!}\left[b_0 + \sum_{j=1}^{k} j!\theta^{-j} f(j)\right].$$

Taking $k = l-2$, $f(k) = -(k+1)b_{2l+1,k+1}/2\Delta$ and $\theta = \alpha\beta/2\Delta$ we obtain

$$b_{2l+1,l-2} = \frac{\left(\frac{\alpha\beta}{2\Delta}\right)^{l-2}}{(l-2)!}\left[b_{5,0} - (l-2)\left(\frac{\alpha\beta}{4\Delta^2}\right)b_{3,0}\right].$$

In general, for $n = l-q$, we should take $k = l-q+1$, $f(k) = -(k+1)b_{2l+1,k+1}/2\Delta$ and $\theta = \alpha\beta/2\Delta$. This results in the expression

$$b_{2l+1,l-q} = \frac{\left(\frac{\alpha\beta}{2\Delta}\right)^{l-q}}{(l-q)!}\sum_{j=0}^{q-1}(-1)^j\mathcal{T}_{l-q}(j)\left(\frac{\alpha\beta}{4\Delta^2}\right)^j b_{2(q-j)+1,0},$$

where $q = 1,2,\ldots,l-1; l = 1,2,\ldots,N$ and the $\mathcal{T}_{l-q}(j)$ are defined as

$$\mathcal{T}_{l-q}(0) = 1;\quad \mathcal{T}_{l-q}(j) = \sum_{s_j=1}^{l-q}\sum_{s_{j-1}=1}^{s_j+1}\cdots\sum_{s_2=1}^{s_3+1}\sum_{s_1=1}^{s_2+1}1 = \frac{(l-q)}{(l-q+2j)}\binom{l-q+2j}{j}.$$

The closed form for $\mathcal{T}_{l-q}(j)$ can be proved by induction on j by noting that

$$\mathcal{T}_{l-q}(k+1) = \sum_{j=2}^{l-q+1}\mathcal{T}_j(k)$$

and using the combinatorial identities

$$\sum_{j=1}^{m}\binom{j+u}{v} = \frac{m+1+u-v}{1+v}\binom{m+u+1}{v} - \frac{1+u-v}{1+v}\binom{u+1}{v}$$

and

$$\sum_{j=1}^{m}j\binom{j+u}{v} = \frac{(m+1+u-v)[m(v+1)-u+v]}{(1+v)(2+v)}\binom{m+u+1}{v} - \frac{(1+u-v)(-u+v)}{(1+v)(2+v)}\binom{u+1}{v}.$$

Therefore, by virtue of (18) and the correspondence $b_{j,n} \to w_{j,n}$, $\lambda_+ \to \lambda_-$, we conclude

$$b_{j,n} = \frac{\left(\frac{\alpha\beta}{2\Delta}\right)^n}{(n-1)!}\sum_{k=0}^{int(j/2)-n-1}\frac{(-1)^k}{2k+n}\binom{2k+n}{k}\left(\frac{\alpha\beta}{4\Delta^2}\right)^k b_{j-2(n+k),0} \tag{20}$$

and

$$w_{j,n} = (-1)^n\frac{\left(\frac{\alpha\beta}{2\Delta}\right)^n}{(n-1)!}\sum_{k=0}^{int(j/2)-n-1}\frac{(-1)^k}{2k+n}\binom{2k+n}{k}\left(\frac{\alpha\beta}{4\Delta^2}\right)^k w_{j-2(n+k),0}. \tag{21}$$

Those $b_{j,n}$ and $w_{j,n}$ described in (16.a) and (16.b) are zero by virtue of the bounds on the summation.

It now remains only to find the $b_{j,0}$ and $w_{j,0}$. Equations (7) and (10.e) linking these objects may be written

$$\begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ \alpha & -\beta/2-\Delta & 0 & 0 \\ 0 & 0 & \alpha & -\beta/2+\Delta \end{pmatrix}\begin{pmatrix} b_{2l,0} \\ b_{2l+1,0} \\ w_{2l,0} \\ w_{2l+1,0}\end{pmatrix} = \begin{pmatrix} P_{2l}(0) - (-1)^l P_1(0) \\ P_{2l+1}(0) - (-1)^l P_1(0) \\ b_{2l+1,1} \\ w_{2l+1,1}\end{pmatrix}. \tag{22}$$

This matrix may be inverted and a recursive solution found for the $b_{2l+1,0}$ and $w_{2l+1,0}$ in terms of the $P_1(0), P_2(0), \ldots, P_{2l+1}(0)$. For the odd $b_{j,0}$ and $w_{j,0}$ one obtains the relations

$$b_{2l+1,0} = \frac{1}{4\Delta}\left\{2\alpha\left[P_{2l}(0) - (-1)^l P_1(0)\right] + (2\Delta-\beta)\left[P_{2l+1}(0) - (-1)^l P_1(0)\right]\right\} - \frac{1}{2\Delta}(b_{2l+1,1} + w_{2l+1}) \tag{23.a}$$

and

$$w_{2l+1,0} = -\frac{1}{4\Delta}\left\{2\alpha\left[P_{2l}(0)-(-1)^l P_1(0)\right]-(2\Delta+\beta)\left[P_{2l+1}(0)-(-1)^l P_1(0)\right]\right\}+\frac{1}{2\Delta}(b_{2l+1,1}+w_{2l+1}). \tag{23.b}$$

We now take (20) and (21) with n set equal to one. Using these relations, together with (24), we take the difference of (23.a) and (23.b) to obtain the recurrence relation

$$(b_{2l+1,0}-w_{2l+1,0}) = \Omega_l - 2\sum_{k=0}^{l-2}\frac{(-1)^k}{2k+1}\binom{2k+1}{k}\left(\frac{\alpha\beta}{4\Delta^2}\right)^{k+1}(b_{2l-2k-1,0}-w_{2l-2k-1,0}),$$

where

$$\Omega_l = \frac{1}{2\Delta}\left\{2\alpha\left[P_{2l}(0)-(-1)^l P_1(0)\right]-\beta\left[P_{2l+1}(0)-(-1)^l P_1(0)\right]\right\}. \tag{24}$$

The solution to this recurrence is

$$(b_{2l+1,0}-w_{2l+1,0}) = \Omega_l - 2\sum_{k=0}^{l-2}(-1)^k\binom{2k+1}{k}\left(\frac{\alpha\beta}{4\Delta^2}\right)^{k+1}\Omega_{l-k-1}.$$

Now that we know the difference $b_{2l+1,0}-w_{2l+1,0}$, using the second line of the matrix (22), we obtain the expressions

$$b_{2l+1,0} = \frac{1}{2}\left[P_{2l+1}(0)-(-1)^l P_1(0)+\Omega_l\right]-\sum_{k=0}^{l-2}(-1)^k\binom{2k+1}{k}\left(\frac{\alpha\beta}{4\Delta^2}\right)^{k+1}\Omega_{l-k-1} \tag{25}$$

and

$$w_{2l+1,0} = \frac{1}{2}\left[P_{2l+1}(0)-(-1)^l P_1(0)-\Omega_l\right]+\sum_{k=0}^{l-2}(-1)^k\binom{2k+1}{k}\left(\frac{\alpha\beta}{4\Delta^2}\right)^{k+1}\Omega_{l-k-1}. \tag{26}$$

To obtain an expression for the even $b_{j,0}, w_{j,0}$ we start by taking the difference

$$\begin{aligned} b_{2l,0}-w_{2l,0} &= \frac{1}{2\Delta}\left\{\beta\left[P_{2l}(0)-(-1)^l P_1(0)\right]+2\alpha\left[P_{2l+1}(0)-(-1)^l P_1(0)\right]\right\} \\ &\quad -\frac{1}{2\Delta\alpha}\left[(\beta-2\Delta)b_{2l+1,1}+(\beta+2\Delta)w_{2l+1,1}\right]. \end{aligned} \tag{27}$$

Now, by evaluating $(\alpha+\lambda_+)(10.e)+(\alpha+\lambda_-)(10.e)_w+\alpha[(10.c)+(10.c)_w]$, where the subscript w means the corresponding w equation, we find that

$$-\frac{1}{2\Delta\alpha}\left[(\beta-2\Delta)b_{2l+1,1}+(\beta+2\Delta)w_{2l+1,1}\right] = -\frac{1}{\Delta}(b_{2l,1}+w_{2l,1})+\frac{\beta}{\Delta}\left[P_{2l-1}(0)-(-1)^{l-1}P_1(0)\right].$$

Therefore (27) becomes

$$(b_{2l,0}-w_{2l,0}) = \Psi_l - 2\sum_{k=0}^{l-2}\frac{(-1)^k}{2k+1}\binom{2k+1}{k}\left(\frac{\alpha\beta}{4\Delta^2}\right)^{k+1}(b_{2l-2k-2,0}-w_{2l-2k-2,0})$$

where

$$\Psi_l = \frac{1}{2\Delta}\left\{\beta\left[P_{2l}(0)-(-1)^l P_1(0)\right]+2\alpha\left[P_{2l+1}(0)-(-1)^l P_1(0)\right]+2\beta\left[P_{2l-1}(0)-(-1)^{l-1}P_1(0)\right]\right\}. \tag{28}$$

Therefore, in an analogous calculation to that for the $b_{2l+1,0}$ and $w_{2l+1,0}$, we find

$$b_{2l,0} = \frac{1}{2}\left[P_{2l}(0)-(-1)^l P_1(0)+\Psi_l\right]-\sum_{k=0}^{l-2}(-1)^k\binom{2k+1}{k}\left(\frac{\alpha\beta}{4\Delta^2}\right)^{k+1}\Psi_{l-k-1} \tag{29}$$

and

$$w_{2l,0} = \frac{1}{2}\left[P_{2l}(0) - (-1)^l P_1(0) - \Psi_l\right] + \sum_{k=0}^{l-2}(-)^k \binom{2k+1}{k}\left(\frac{\alpha\beta}{4\Delta^2}\right)^{k+1}\Psi_{l-k-1}. \tag{30}$$

We are now in possession of the coefficents which define the solution to our example rate matrix A. Specifically, the coefficents $a_{j,1}$ and $a_{j,2}$ are given by (9.d) and (9.e), the $b_{j,n}$ and $w_{j,n}$ by (20) and (21), and the $b_{j,0}$ and $w_{j,0}$ by (24), (25), (26), (28), (29) and (30). The advantage of this method over reduction to Jordan canonical form of the matrix A is now clear. The Jordan form calculation must be done anew for each larger value of N, with the problem becoming quickly intractible as the dimension of the matrix A is increased. The solution derived in this paper is exact, for arbitrary N.

4 An Application to Spin Pumping

It is instructive to consider the similarities between our example set of ODE's and the set of equations generated in the study of spin pumping and relaxation problems in nuclear physics. We now look at the approximation $\beta \ll \alpha$. In this limit our expressions derived in Section 3.2 greatly simplify to give the time dependent populations $P_j(t)$ in terms of the initial values of these populations.

The problem we describe arises in the study of transitions between spin states in a system with a nucleus of spin F and a single orbital electron of spin $S = \frac{1}{2}$. An example of an $F = \frac{1}{2}$ system is the hydrogen atom, and of an $F = 0, 1$ system is neutral muonic Helium-3. We define $J = F + S$ to be the total spin of the system, and take the component of the spins in an arbitrarily chosen direction to be F_z, S_z and J_z. For a given value of F, the total number of spin states is $4F + 2$.

We now introduce two types of transition which may occur; a spin pumping linking states of the same F_z yet different S_z, and a mixing of states of the same J_z. The spin pumping is externally imposed and takes the form of a spin-transfer interaction with laser-polarized alkali-metal atoms [3]. The spin pumping rate is equivalent to the rate β in our model and is taken to be constant for all F_z.

The physics of the mixing interaction is as follows. A pair of states with the same J_z may be represented by orthogonal basis wavefunctions labelled either by the quantum numbers F_z and S_z, or by the quantum numbers J and J_z. These two sets of basis functions may be written as $|F_z \quad S_z\rangle$ and $|J \quad J_z\rangle$. The states of definite J and J_z are energy eigenstates, with respect to the mixing interaction. The observed states are, however, states of definite F_z and S_z, giving rise to the state mixing.

In the remainder of this section the population $P_j(t)$ corresponds to the state with quantum numbers F, F_z and S_z such that $j = 2F + 2F_z + S_z + \frac{3}{2}$. Figure 1 is an explicit portrayal of the system with $S = \frac{1}{2}$, $F = 2$. The vertical arrows represent a spin transfer that proceeds at a rate β while the diagonal slashes depict a mixing interaction of rate α. This gives a rate matrix identical to that of (2).

This assumption that the mixing interaction may be characterized by a unique parameter α, for all values of J_z, is where the similarity breaks down between the physical situation and the example of Section 3. In the physical problem, this uniqueness of α would imply that the vector coupling coefficients linking the states $|F_z \quad S_z\rangle$ and $|J \quad J_z\rangle$ are the same for all J_z. This is only the case for the $F = \frac{1}{2}$ situation. For all larger values of F we should expect the results of Section 3 to be quite different from the measured populations of the physical case.

With this limitation in mind, we proceed to calculate the time dependencies of the populations for an arbitrary value of N, where we take the nuclear spin $F = \frac{1}{2}N$. A useful experimentally measured quantity is a combination of the populations called the vector polarization, defined by

$$P_V(t) \equiv P_{2N+2}(t) + P_{2N+1}(t) - P_2(t) - P_1(t).$$

For $\beta = 0$, our model predicts that

$$P_V(t)|_{\beta=0} = \frac{1}{2}\left[2P_{2N+2}(0) + P_{2N+1}(0) + P_{2N}(0) - P_3(0) - P_2(0) - 2P_1(0)\right]$$
$$+\frac{1}{2}\left[P_{2N+1}(0) - P_{2N}(0) + P_3(0) - P_2(0)\right]e^{-2\alpha t}.$$

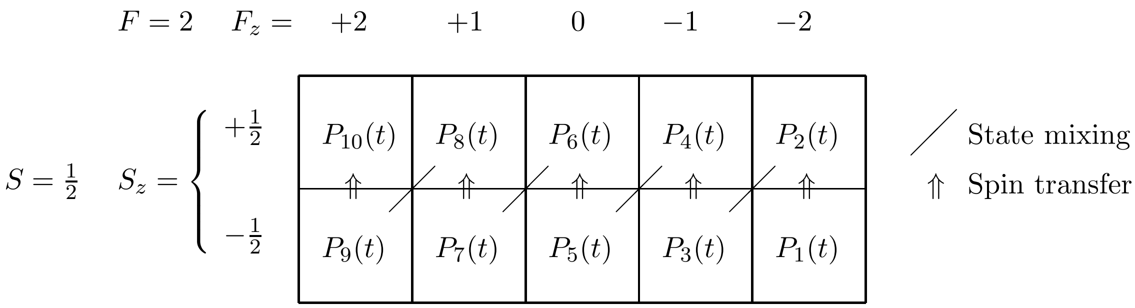

Figure 1: The spin transfer and state mixing interactions are shown in relation to the spin populations $P_j(t)$.

A quantum mechanical determination of $P_V(t)$ with $\beta = 0$, $P^{QM}_{V,\beta=0}(t)$ can be done exactly. If we further suppose that the initial populations are set equal and normalized so that $P^{QM}_{V,\beta=0}(0)$, then $P^{QM}_{V,\beta=0}(t) = 0$ for all t. This implies that it would be consistent with the physical picture if we were to choose the initial conditions of our model such that $P_j(0) = 1/(2N+2)$ for all j. This uniquely defines the vector polarization predicted by our model when $\beta \neq 0$. The condition $\beta \ll \alpha$ is equivalent to the justified approximation that, in suitable units, the spin pumping rate is very much slower than the mixing rate which is characterized by the energy splitting between states of equal J_z. With this approximation our model predicts that

$$P_V(t) \simeq \left(1 - e^{-\frac{\beta t}{2}}\right) - e^{-\frac{\beta t}{2}} \sum_{n=1}^{N-1} \frac{1}{n!} \left(\frac{\beta t}{2}\right)^n \frac{N-n}{N+1}. \tag{31}$$

In comparison, an empirically motivated form for the vector polarization [4] is

$$P^{exp}_V(t) = 1 - e^{-f_\eta \beta t}$$

where

$$f_\eta = \frac{3}{(N+1)^2 + 2}.$$

This expression matches our formula exactly for $F = \frac{1}{2}$ $(N = 1)$ but, due to the differences noted earlier between the model and this physical situation, shows a rather longer rise-time for higher F states. The empirical form $P^{exp}_V(t)$ has been used as a comparison, since we do not know of any exact theoretical expression for the time-dependent vector polarization.

5 Conclusions

We have generated an exact solution to a system of linear ODE's whose associated rate matrix exhibits a high degree of degeneracy in its eigenvalues. The solutions are constructed by solving a number of non-trivial recurrence relationships. This method of solution easily generalizes to any rate matrix provided its eigenvalues have high multiplicity. These solutions allow one to carefully analyze the analytic behaviour of a system of degenerate ODE's as the dimension of the system increases. Expressions which are functions of the dimension of the system's degeneracy may be generated, such as (31) of the previous section. This is in contrast to the results of more traditional methods of solution, such as reduction to Jordan canonical form. In that case, such results would have to be independently derived for each larger rate matrix, the method quickly becoming intractible for all but the most trivial cases.

References

[1] S. L. Campbell, *Singular Systems of Differential Equations*, Research Notes in Mathematics, Vol. **40**, Pitman, 1980.

[2] S. I. Grossman, *Elementary Linear Algebra*, Wadsworth, 1987.

[3] H. R. Cole and R. E. Olson, *Spin-exchange cross sections for hydrogen-atom – alkali-metal-atom collisions,* Phys. Rev. A **31**, 2137 (1985).

[4] G. D. Cates et al., *Lampf Research Proposal Number 1231,* Nov. 1990.