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A Diagrammatic Mnemonic for Calculation of Cascading Level Populations

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A diagrammatic procedure is described, by which the time dependence of the population of any level in a decay scheme of arbitrary complexity can be prescribed directly in terms of transition probabilities and initial populations, without specifically solving the determining differential equations.

INTRODUCTION

Many problems in atomic and nuclear physics are concerned with quantum energy levels which decay downward at a rate proportional to the population of the decaying level. The instantaneous population of a given level is determined by its transition probabilities, as well as the transition probabilities and populations of the levels above it which, either directly or indirectly, decay into it. Thus, the population of a given level can be determined as a function of time, initial populations, and transition probabilities by the solution of a set of coupled differential equations. Special solutions of these differential equations, with only one or two contributing upper levels, or with only a few nonvanishing initial populations and transition probabilities, are presented in many textbooks on elementary nuclear chemistry,[1,2] and in many recent research reports on atomic spectroscopy.[3,4] For complicated decay schemes, the calculation is straightforward but can become very tedious.

It is possible to write the population equation for any decay scheme as a decomposition into the individual cascade contributions, grouped according to the number of steps in the cascade. All members of such a group correspond to the same generic cascade diagram, and have the same generic solution in terms of general level parameters. The solution for a specific decay scheme can be formed by summing the solutions corresponding to all possible cascade diagrams within the decay scheme in question. Thus, the time dependence of the population of any level in a decay scheme of arbitrary complexity can be prescribed directly in terms of transition probabilities and initial populations, without specifically solving the determining differential equations.

Exposition of the cascading decay process in this manner not only provides a mnemonic for prescribing level populations, but is also of pedagogic value, since it permits a complex mechanism to be visualized as a large number of simple and independent mechanisms proceeding simultaneously.

I. MATHEMATICAL SOLUTION

Consider a set of levels labeled consecutively in increasing order of energy from 1 to m. The population at time t of the jth level is denoted $N_j(t)$, and the transition probability between levels j and k is denoted A_{jk}. The differential equation for the population of the nth level is given by

$$dN_n/dt=\sum_{i=n+1}^{m} N_i(t)A_{in}-N_n(t)\sum_{f=1}^{n-1}A_{nf}. \quad (1)$$

The decay constant α_j (the inverse of the mean-life) of the level j is defined as the sum of the transition probabilities between the level j and all levels below it.

$$\alpha_j=\sum_{f=1}^{j-1}A_{jf}. \quad (2)$$

The differential Eq. (1) can be converted to an integral equation by use of the integrating factor $\exp(\alpha_n t)$. Performing the integration and exchanging the orders of integration and summation, the

[1] I. Kaplan, *Nuclear Physics* (Addison–Wesley Publ. Co., Inc., Reading, Mass., 1963), Chap. 10.
[2] R. D. Evans, *The Atomic Nucleus* (McGraw-Hill Book Co., New York, 1955), Chap. 15.
[3] W. S. Bickel and A. S. Goodman, Phys. Rev. **148**, 1 (1966).
[4] M. R. Lewis *et al.*, Phys. Rev. **164**, 94 (1967).

integral equation for the population of level n is

$$N_n(t) = \exp(-\alpha_n t)\left[N_n(0) + \sum_{i=n+1}^{m} A_{in} \int_0^t dt' \exp(\alpha_n t') N_i(t')\right]. \tag{3}$$

Since the level population occurs on both sides of the equality, the equation can be successively iterated to yield a finite (for finite m) series of nested sums and nested integrals. The iterated expression becomes

$$\begin{aligned} N_n(t) = \exp(-\alpha_n t) \Bigg\{ & N_n(0) + \sum_{i=n+1}^{m} N_i(0) A_{in} \int_0^t dt' \exp[(\alpha_n - \alpha_i)t'] \\ & + \sum_{i=n+1}^{m-1} \sum_{j=i+1}^{m} N_j(0) A_{ji} A_{in} \int_0^t dt' \exp[(\alpha_n - \alpha_i)t'] \int_0^{t'} dt'' \exp[(\alpha_i - \alpha_j)t''] \\ & + \sum_{i=n+1}^{m-2} \sum_{j=i+1}^{m-1} \sum_{k=j+1}^{m} N_k(0) A_{kj} A_{ji} A_{in} \int_0^t dt' \exp[(\alpha_n - \alpha_i)t'] \\ & \times \int_0^{t'} dt'' \exp[(\alpha_i - \alpha_j)t''] \int_0^{t''} dt''' \exp[(\alpha_j - \alpha_k)t'''] + \text{etc.} \Bigg\}. \end{aligned} \tag{4}$$

This series has several interesting features. First, all integrals are standard exponential forms and can be performed exactly. Second, the order of each term is specified both by the depth of nesting and the number of transition probability product factors. Third, the lower limits of the more deeply nested sums restrict the upper limits of sums of shallower nesting within a given term. Thus, the series terminates with the term of order $(m-n)$, where the upper and lower limits coincide.

A physical interpretation can be achieved by noticing that each order of the series in Eq. (4) contains all those cascades which move from initial levels to the level of interest in a number of steps equal to the order of the term. To emphasize this identification we denote each order by a sum of labeled diagrams, enclosed in curly brackets, which depict the cascade appropriate to that order. This diagrammatic statement of the population Eq. (4) is shown in Fig. 1.

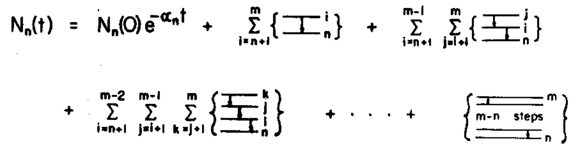

FIG. 1. Diagrammatic decomposition of a level population into its cascade contributions.

Comparing Fig. 1 with Eq. (4), it is clear that each diagram represents a well-defined and exactly integrable expression. The expression is generic to its diagrammatic order and can be computed in terms of transition probabilities and initial populations of arbitrarily labeled contributing levels. Further, these expressions can be canonically formed for arbitrary order.[5] The diagrammatic expressions for the first, second, third, and $(m-n)$th orders are tabulated below. (The diagrammatic symbols are written serially for typographic purposes.)

$$\{i \to n\} = N_i(0) A_{in} [\exp(-\alpha_i t)/(\alpha_n - \alpha_i) + \exp(-\alpha_n t)/(\alpha_i - \alpha_n)]. \tag{5}$$

$$\begin{aligned} \{j \to i \to n\} = N_j(0) A_{ji} A_{in} [& \exp(-\alpha_j t)/(\alpha_i - \alpha_j)(\alpha_n - \alpha_j) + \exp(-\alpha_i t)/(\alpha_j - \alpha_i)(\alpha_n - \alpha_i) \\ & + \exp(-\alpha_n t)/(\alpha_j - \alpha_n)(\alpha_i - \alpha_n)]. \end{aligned} \tag{6}$$

$$\begin{aligned} \{k \to j \to i \to n\} = N_k(0) A_{kj} A_{ji} A_{in} [& \exp(-\alpha_k t)/(\alpha_j - \alpha_k)(\alpha_i - \alpha_k)(\alpha_n - \alpha_k) \\ & + \exp(-\alpha_j t)/(\alpha_k - \alpha_j)(\alpha_i - \alpha_j)(\alpha_n - \alpha_j) + \exp(-\alpha_i t)/(\alpha_k - \alpha_i)(\alpha_j - \alpha_i)(\alpha_n - \alpha_i) \\ & + \exp(-\alpha_n t)/(\alpha_k - \alpha_n)(\alpha_j - \alpha_n)(\alpha_i - \alpha_n)]. \end{aligned} \tag{7}$$

$$\{m \to \cdots \to n\} = N_m(0) \left[\prod_{i=n}^{m-1} A_{i+1\,i}\right] \sum_{j=n}^{m} [\exp(-\alpha_j t) / \prod_{k \neq j} (\alpha_k - \alpha_j)]. \tag{8}$$

[5] H. Bateman, Proc. Cambridge Phil. Soc. 15, 423 (1910).

Thus, the solution to a specific problem is reduced to counting and labeling all possible cascade diagrams of each order contained in the decay scheme of that problem, and substituting the appropriately labeled canonical expression for each diagram. The technique is best illustrated by a sample calculation.

II. SAMPLE CALCULATION

As an example of this technique, let us compute the population of a level (denoted by 3) which is fed by three upper levels (denoted by 4, 5, 6) and which decays into two lower levels (denoted by 1, 2). The level scheme, with the transitions contributing to the population of level 3 indicated according to the order of the cascade, is shown in Fig. 2.

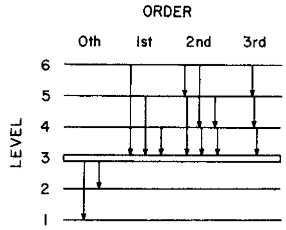

FIG. 2. Sample decay scheme, with the transitions contributing to the population of level 3 indicated according to the order of the cascade.

Summing all possible diagrams which can cascade into level 3, the population is represented by

$$N_3(t)=N_3(0)\exp(-\alpha_3 t)+\{6\to3\}+\{5\to3\}+\{4\to3\}+\{6\to5\to3\}+\{6\to4\to3\}+\{5\to4\to3\}+\{6\to5\to4\to3\}. \quad (9)$$

Substituting the appropriately labeled canonical expression corresponding to each diagram,

$$\begin{aligned}N_3(t)=&N_3(0)\exp(-\alpha_3 t)+N_6(0)A_{63}\left[\frac{\exp(-\alpha_6 t)}{(\alpha_3-\alpha_6)}+\frac{\exp(-\alpha_3 t)}{(\alpha_6-\alpha_3)}\right]\\
&+N_5(0)A_{53}\left[\frac{\exp(-\alpha_5 t)}{(\alpha_3-\alpha_5)}+\frac{\exp(-\alpha_3 t)}{(\alpha_5-\alpha_3)}\right]+N_4(0)A_{43}\left[\frac{\exp(-\alpha_4 t)}{(\alpha_3-\alpha_4)}+\frac{\exp(-\alpha_3 t)}{(\alpha_4-\alpha_3)}\right]\\
&+N_6(0)A_{65}A_{53}\left[\frac{\exp(-\alpha_6 t)}{(\alpha_5-\alpha_6)(\alpha_3-\alpha_6)}+\frac{\exp(-\alpha_5 t)}{(\alpha_6-\alpha_5)(\alpha_3-\alpha_5)}+\frac{\exp(-\alpha_3 t)}{(\alpha_6-\alpha_3)(\alpha_5-\alpha_3)}\right]\\
&+N_6(0)A_{64}A_{43}\left[\frac{\exp(-\alpha_6 t)}{(\alpha_4-\alpha_6)(\alpha_3-\alpha_6)}+\frac{\exp(-\alpha_4 t)}{(\alpha_6-\alpha_4)(\alpha_3-\alpha_4)}+\frac{\exp(-\alpha_3 t)}{(\alpha_6-\alpha_3)(\alpha_4-\alpha_3)}\right]\\
&+N_5(0)A_{54}A_{43}\left[\frac{\exp(-\alpha_5 t)}{(\alpha_4-\alpha_5)(\alpha_3-\alpha_5)}+\frac{\exp(-\alpha_4 t)}{(\alpha_5-\alpha_4)(\alpha_3-\alpha_4)}+\frac{\exp(-\alpha_3 t)}{(\alpha_5-\alpha_3)(\alpha_4-\alpha_3)}\right]\\
&+N_6(0)A_{65}A_{54}A_{43}\left[\frac{\exp(-\alpha_6 t)}{(\alpha_5-\alpha_6)(\alpha_4-\alpha_6)(\alpha_3-\alpha_6)}+\frac{\exp(-\alpha_5 t)}{(\alpha_6-\alpha_5)(\alpha_4-\alpha_5)(\alpha_3-\alpha_5)}\right.\\
&\left.+\frac{\exp(-\alpha_4 t)}{(\alpha_6-\alpha_4)(\alpha_5-\alpha_4)(\alpha_3-\alpha_4)}+\frac{\exp(-\alpha_3 t)}{(\alpha_6-\alpha_3)(\alpha_5-\alpha_3)(\alpha_4-\alpha_3)}\right]. \quad (10)\end{aligned}$$

Since levels 1 and 2 occur only through the sum $\alpha_3=A_{31}+A_{32}$, the expression is valid for any multiplicity of levels below level 3. Notice that the time dependence of (10) resides in four exponential decay terms: one for the level of interest, and one for each level cascading into it. By regrouping and factoring, the coefficient of each exponential can be written in terms of initial populations and transition probabilities.