

A Note on Integro-Differential Explicit Method of the Master Equation Solution

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Abstract

A new theoretical approach is presented for solving the master equation of nuclear preequilibrium states, based on an explicitly integrated method. Earlier *ad hoc* hypothesis was proposed to follow mathematical derivation of the master equation reasonably, thus providing an explicit method to derive the dependence of probability distributions of exciton levels occupation. Few theoretical comparisons were made, based on approximation formulae of the present solution.

1. Introduction

The preequilibrium models represent a group of models that try to describe the intermediate nuclear reactions based on the contribution weight of many statistical states in each reaction channel. A model with significance is the exciton model [1-4], which depicts intermediate stages of nuclear reactions based on excitations occurring due to development of residual two-body interaction. The exciton model implies that a hypothetically and temporarily created entity, *the exciton*, a notion for particle-hole (p, h) pair, is responsible of this development. The idea was first described by Griffin [4]. Intermediate states of interaction will ensure that the *number of excitons* n ($=p+h$) distinguishing each stage in the equilibration process will change by an even integer, that is $\Delta n = \pm 2$ or zero. At every stage in this course, equilibration is specified by an n and excitation energy E , both of which will affect a certain decay probability W . Transition between adjacent stages is characterized by the transition rate, λ_{a-b} between stages a and b as given by Fermi rule, depending on the matrix element of the interaction [2].

During exciton model calculations, the master equation ME, will describe the time evolution of occupation probability of each stage based on a first order differential equation. It expresses various states development at a given time. In [1,5] a comprehensive review and solution methods of ME description was given. ME in

terms of one-component system, when protons and neutrons are approximated to have the same behavioral characteristics, is given as [6]

$$\frac{dP(n, E, t)}{dt} = \lambda_{n+2}^-(n, E) P(n+2, E, t) + \lambda_{n-2}^+(n, E) P(n-2, E, t) - \frac{P(n, E, t)}{\tau_n(n, E)} \quad (1),$$

where $P(n, E, t)$ is the occupation probability of the n^{th} stage with E at t , and λ^+, λ^- are adjacent transition rates with resp. The mean lifetime of this stage τ_n is

$$\tau_n(n, E) = \left(\lambda_n^-(n, E) + \lambda_n^+(n, E) + W(n, E) \right)^{-1} \quad (2),$$

and $W(n, E)$ is the exciton rate of decay to the continuum. The total lifetime for each state is given by

$$T(n, E) = \int_0^{\infty} P(n, E, t) dt \quad (3),$$

For two-component system of reaction where neutrons are distinguished from protons, the ME is given as [5]

$$\begin{aligned} \frac{dP(N, h_{\pi}, t)}{dt} = & \left[\lambda_{v\pi}^{++}(E, N-1, h_{\pi}) + \lambda_{\pi\pi}^{++}(E, N-1, h_{\pi}) \right] P(N-1, h_{\pi}-1, t) \\ & + \left[\lambda_{\pi v}^{+0}(E, N-1, h_{\pi}) + \lambda_{v v}^{+0}(E, N-1, h_{\pi}) \right] P(N-1, h_{\pi}, t) \\ & + \left[\lambda_{v v}^{-0}(E, N+1, h_{\pi}) + \lambda_{\pi v}^{-0}(E, N+1, h_{\pi}) \right] P(N+1, h_{\pi}, t) \\ & + \left[\lambda_{\pi\pi}^{-}(E, N+1, h_{\pi}+1) + \lambda_{v v}^{-}(E, N+1, h_{\pi}+1) \right] P(N+1, h_{\pi}+1, t) \\ & + \left[\lambda_{v\pi}^{0+}(E, N, h_{\pi}-1) \right] P(N, h_{\pi}-1, t) \\ & + \left[\lambda_{\pi v}^{0-}(E, N, h_{\pi}+1) \right] P(N, h_{\pi}+1, t) \\ & - \left[\lambda_{\pi v}^{+0}(E, N, h_{\pi}) + \lambda_{v v}^{+0}(E, N, h_{\pi}) + \lambda_{v\pi}^{++}(E, N, h_{\pi}) \right. \\ & + \lambda_{\pi\pi}^{++}(E, N, h_{\pi}) + \lambda_{v v}^{-0}(E, N, h_{\pi}) + \lambda_{\pi v}^{-0}(E, N, h_{\pi}) \\ & + \lambda_{\pi v}^{-}(E, N, h_{\pi}) + \lambda_{\pi\pi}^{-}(E, N, h_{\pi}) + \lambda_{v\pi}^{0+}(E, N, h_{\pi}) \\ & \left. + \lambda_{\pi v}^{0-}(E, N, h_{\pi}) + W(E, N, h_{\pi}) \right] \times P(N, h_{\pi}, t) \quad (4), \end{aligned}$$

where n_{π}, n_v are the exciton numbers for protons and neutrons, respectively, $n = n_{\pi} + n_v$ and $P(N, h_{\pi}, t)$ of n_{π}, n_v number of excitons. N is a function of n_{π}, n_v number as: $n = p_{\pi} + h_{\pi} + p_v + h_v = 2(N+1) + n_o$, and n_o is the initial exciton number. h

and p represent hole and particle numbers, and the subscripts π, ν represent proton and neutron types, respectively. The decay rate $W(N, h_\pi)$ is defined as [7],

$$W(N, h_\pi) = \sum_{\beta} W_{\beta}(N, h_\pi) d\varepsilon \quad (5),$$

and $W(N, h_\pi)$ is the decay rate of a particle of type β to the continuum with energy ε from the state described by N and h_π . This problem is of major significance in preequilibrium models, specially the exciton model [8-10].

In the present work we provide a note on the solution of eq.(4), which is applied for a ne solution of the two-component ME.

2. Theory: The Integro-Differential Master Equation

If one examines eq.(4), it can be shown that it is equivalent to,

$$\frac{dP'(t)}{dt} = \sum_{j=1}^{10} \lambda_j P_j(t) - \left(\sum_{j=1}^{10} \lambda'_j + W \right) P'(t) \quad (6).$$

where an assumption was made that various population probabilities are,

$P(N, h_\pi) = P'_1 = P'_2 = P'_3 = \dots = P'_{10} = P'_{11} = P'$, and the prime (magnified acute accent) sign is added in order to distinguish these (successive) probabilities from (initial) P , the prime here *does not* mean a derivative operation. Eq.(6) is ME rewritten in a compact form. Noting that λ'_j 's are not functions of t , neither is W , then we'll further define the following,

$$B(t) = \sum_{j=1}^{10} \lambda_j P_j(t) \quad (7),$$

$$A = \sum_{j=1}^{10} \lambda'_j + W \quad \neq (A(t)) \quad (8),$$

then eq.(6) can simply be turned to,

$$\frac{dP'(t)}{dt} + A P'(t) = B(t) \quad (9).$$

Let's define, $P'(t) = uv$, where u and v are partial functions of P , and let us assume a general form of $v = \exp(-At)$, this definition of v implies that $\frac{dv}{dt} + Av = 0$, thus,

$P_j(t=0) = P_{o_j} = k = \text{constant}$ and one may write,

$$B(t=0) = B_o = \sum_j^{10} \lambda_j k \tag{10}$$

after few steps,

$$P'(t) = \exp(-At) \int_{t'=0}^t \exp(At') B(t') dt' + P'_o \exp(-At) \tag{12}$$

where $P'_o = P'(t=0)$. This is the integrated form of ME. The exponential function was added here to describe a general behavior of nuclear decay. It is consistent with the results of the simpler one-component ME system found in [1].

2.1. The Solution:

The importance of eq.(12) is seen here because it was given in a form that can be solved analytically. In previous methods of ME solution, no direct expression for the probability distribution $P'(t)$ was given, but instead, only the integral form of $P'(t)$ is usually reached that is similar to eq.(12) -see [1] for detailed survey on solution methods of ME.

Let us try to rewrite eq.(6) again as,

$$\frac{dP_k}{dt} = \sum_{j=1}^{S_j} \lambda_{j,k} P_j - \sum_{j=1}^{S_j} \lambda_{k,j} P_k - W_k P_k \tag{13}$$

where $\lambda_{j,k}$ is transition rate from the state j to the state k and S_j in the summation limit is the number of states surrounding the j^{th} state, without including the j^{th} state itself, because there is no transition from the j^{th} state to itself. Note that here the index k has a similar meaning given by Herman et al.[6] for index representation,

$$k = \frac{(n - n_o)(n - n_o + 2)}{8} + h_\pi + 1, \text{ and it leads to the scheme shown in Fig.(1).}$$

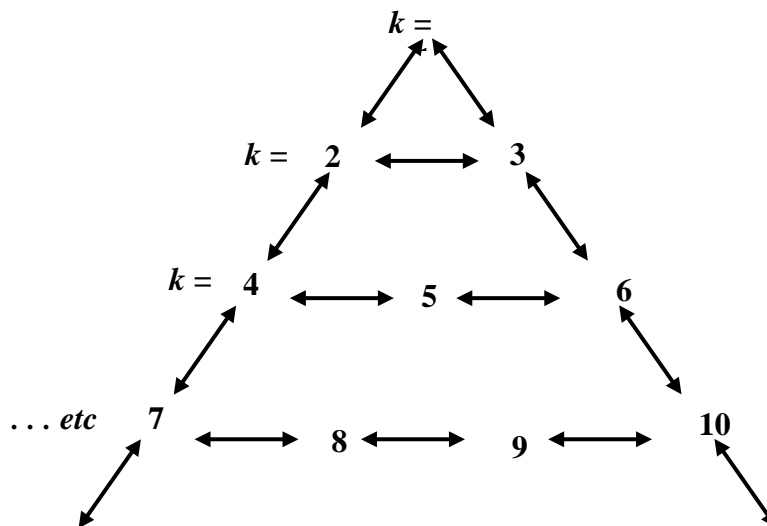


Fig.(1). A scheme representing the transition from various states.

To put eq.(13) in general form let us define Δ_{jk} as,

$$\Delta_{jk} = 1 - \delta_{jk} = \begin{cases} 0 & j = k \\ 1 & j \neq k \end{cases} \quad (14),$$

where δ_{jk} is the usual Kronecker delta function. Obviously,

$$\Delta_{jk} = \Delta_{kj} \quad (15).$$

Then eq.(13) can be safely written as follows,

$$\frac{dP_k}{dt} = \sum_{j=1}^{S_j} \Delta_{jk} \lambda_{j,k} P_j - \left[\sum_{j=1}^{S_j} \Delta_{jk} \lambda_{k,j} + W_k \right] P_k \quad (16).$$

As before we put the definitions of B_k and A_k as follows,

$$B_k = \sum_{j=1}^{S_j} \Delta_{jk} \lambda_{j,k} P_j \quad (17-a),$$

$$A_k = \sum_{j=1}^{S_j} \Delta_{kj} \lambda_{k,j} + W_k \quad (17-b),$$

here S_j represents all the states surrounding the j^{th} state with no restrictions, because we added the analytical function Δ_{kj} which forces this conditions as a selection rule since $\Delta_{kj} = 0$ when $k = j$. Eq.(13) is now equivalent to,

$$\frac{dP_k}{dt} = B_k - A_k P_k \tag{18},$$

and eq.(12) becomes,

$$P_k = \exp(-A_k t) \int_{t'=0}^t \exp(A_k t') B_k dt' + P_{ok} \exp(-A_k t) \tag{19}.$$

Once again, the functions A_k is not a function of time. t' also is used for integration purpose only. The solution of the explicitly-integrated form of the master equation is given below. To integrate eq.(19) let's define part of the integral as,

$$I = \sum_{j=1}^{S_j} \Delta_{jk} \lambda_{j,k} \int_{t'=0}^t \exp(A_k t') P_j(t') dt', \tag{20}.$$

Then after few steps,

$$P_k = \frac{\sum_j \Delta_{jk} \lambda_{j,k} P_j}{A_k} + P_{ok} \exp(-A_k t) - \frac{\sum_j \Delta_{jk} \lambda_{j,k} A_j}{A_k} \times \left(T_\ell - T_j - A_k \exp(-A_k t) \int \exp(A_k t) (T_\ell - T_j) dt \right) - W_j \exp(-A_k t) \int P_\ell \exp(A_k t) dt \tag{21},$$

which represents the explicit solution of ME. The ℓ^{th} stat is presented to differ from

the j^{th} one, from defining $B_j = \sum_{\ell=1}^{S_j} \Delta_{\ell j} \lambda_{\ell,j} P_\ell$ and $A_j = \sum_{\ell=1}^{S_j} \Delta_{\ell j} \lambda_{j,\ell} + W_j$. Eq.(21) was

derived without approximation. Apparently, the first difficulty faced is the integrations of T 's in the second and third terms.

2.2. Approximations

However, one may apply some approximations at this point because of the significant and specific shape of eq.(21). As a first approximation let the equilibration time t_{eq} be long enough so that the exponentials with negative exponents fall fast with time, and W are not significant at each stage, and let the mean lifetimes of adjacent stages be almost equal, i.e., $T_\ell \approx T_j$ and $W_j \exp(-A_k t) \approx 0$. Then $P_k = \frac{B_j}{A_k} + P_{ok} \exp(-A_k t)$, thus $P_k \propto P_j$. This means that the occupation probability of the state k relates to all occupation probabilities of the surrounding j^{th} states because every k^{th} state is actually a newly born daughter and a mother of the surrounding states at the same time which is the idea of detailed balance behind ME. The proportionality above is therefore an image taken from eq.(5).

At small values of time, then if one accepts the approximation $\sum \Delta_{jk} \lambda_{j,k} / \left(\sum \Delta_{jk} \lambda_{j,k} + W_j \right) \approx 1$ which means that W is much smaller (in magnitude) than the sum of transition rates then one can have, $P_k \cong P_j + P_k(t=0) \exp(-A_k t)$.

3. Discussions and Conclusion

The physical interpretation of eq.(13) ensures that for stage with $k=1$ (first stage), the following approximation holds, $\exp(-A_1 t) \int_{t'} \exp(A_1 t') B_1 dt' \cong 0$ because the first stage mainly gives to other stages, its chance to receive from other stages is almost zero. Thus, $P_1 \cong P_{o1} \exp(-A_1 t)$ which is very similar to the well-known nuclear decay $N = N_o \exp(-\lambda t)$, noting that in here $A = \sum_j \lambda_j$. Therefore we choose the expression $P_{ok} \exp(-A_k t)$ rather than P_{ok} only. One should be careful how to apply and use the

approximation above because we have, $\exp(A_1 t) \sum_{j=1}^3 \Delta_{j1} \lambda_{j,1} P_j = \text{constant} = \beta_1 \exp(-A_1 t)$

where $\beta \neq B$. Thus we'll have,

$$\sum_{j=1}^3 \Delta_{j1} \lambda_{j,1} P_j = \beta_1 \exp(-A_1 t) \tag{22}.$$

Now if we take the time derivative for both sides of eq.(22) then,

$$\beta_1 \exp(-A_1 t) = \frac{-1}{A_1} \sum_{j=1}^3 \Delta_{j1} \lambda_{j,1} \frac{dP_j}{dt} \tag{23},$$

and from this we have,

$$\sum_{j=1}^3 \Delta_{j1} \lambda_{j,1} \left[\frac{1}{A_1} \frac{dP_j}{dt} + P_j \right] = 0 \tag{24},$$

and clearly this equation holds if $(\frac{1}{A_1} \frac{dP_j}{dt} + P_j) = 0$, $\lambda_{j,1} = 0$, or $j=1$; all of which will logically lead to, $P_j = P_{oj} \exp(-A_1 t)$, ($j = 2$ and 3 only) which is the exact form of eq.(24) for $j=1$. Eq.(21) will lead to the solution of all stages with the same form, *i.e.*, will give a solution of the type, $P_j = P_{oj} \exp(-A_1 t)$, for all values of j and also it reveals that $P'(t) = uv$ actually reduced to $P'(t) = v$, and this isn't quite efficient as a full solution, but it is an approximation. Therefore eq.(21) must be handled with care as being for the case with $j=1$ only because is not valid for all stages of the preequilibrium reaction, but the more reasonable form, eq.(19) is always valid which is a useful relation that describes the population probability of the k^{th} state is the same of the j^{th} state plus the initial population of the same k^{th} state, which decreases exponentially with time t . Therefore, the asymptotic behavior of the k^{th} occupation probability will directly be as $P_k = P_j$ and this is the situation that describes the equilibration condition.

A third point seen from the above eq.(21) is that, if one assumed that initially $P_j = 0$, which means that all surrounding states are empty. Then $P_k = P_k(t=0) \exp(-A_k t)$,

and this again is the well-known decay law of any excited equilibrated, or compound nucleus. In the case of $P_j = 0$ then we will have no j^{th} states, therefore there will be no transition rates from or to these states and we must set all λ_j to zero, *i.e.*, we will have $A_k = W_k$ only. This leads immediately to have a solution form as $P_k = P_k(t=0) \exp(-W_k t)$, simply, if we labeled W by λ , and $P_k(t=0)$ by P_0 , then we write $P = P_0 \exp(-\lambda t)$, the natural radioactive decay law.

To compare with earlier *ad hoc* hypothesis, Griffin [4] put the following formula -the same symbols are used as found in Ref.4 for convenience,

$$P_p^{(E)} dE = \frac{\sum_n \rho_{n-1}^{(u)} \rho_n(E)}{\sum_n \rho_{n-1}} dE,$$

and Blann [10, 11] put the following,

$$P_x(E) dE = \sum_{n=n_0}^{\hat{n}} n f_x \left[\frac{\rho_{n-1}(U)}{\rho_n(E)} \right] \left[\frac{\lambda_c(E)}{\lambda_c(E) + \lambda_{n+2}(E)} \right] D_n$$

where $\rho_n(E)$ is the density of states with exciton number n and energy E , $n f_x$ is the emission ratio of a particle of type x , $\lambda_c(E)$ is the decay rate to the continuum, *i.e.*,

$\lambda = W$, and $D_n = \prod_{n'=n_0+2}^n (1 - P_{n'-2})$. In this paper we've tried to find an analytical

reason behind this assumption. Comparing Blann's [11] result in particular

$$\frac{\lambda_c}{\lambda_c + \lambda_{n+2}} \left(\prod_{n'} (1 - P_{n'-2}) \right) \text{ with our approximation } \frac{\sum \Delta_{jk} \lambda_{j,k}}{\left(\sum \Delta_{jk} \lambda_{j,k} + W_j \right)} \approx 1$$

a general analogy is seen, as both have ratio of transition rates multiplied by probability function, and the definition of Δ compensates for the term inside the multiplication procedure.

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