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Synergetics

An Introduction

Nonequilibrium Phase Transitions and Self-Organization in Physics, Chemistry, and Biology

Third Revised and Enlarged Edition

With 161 Figures

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To the Memory of

Maria and Anton Vollath

4.5 The Master Equation

This section can be read without knowledge of the preceding ones. The reader should be acquainted, however, with the example of Section 4.2. The master equation we shall derive in this chapter is one of the most important means to determine the probability distribution of a process. In Section 4.2 we have already encountered the example of a particle which is randomly pushed back or forth. Its motion was described by a stochastic equation governing the change of the probability distribution as a function of time. We will now consider the general case in which the system is described by discrete variables which can be lumped together to a vector $\boldsymbol{m}$. To visualize the process think of a particle moving in three dimensions on a lattice.

The probability of finding the system at point $\boldsymbol{m}$ at a time t increases due to transitions from other points $\boldsymbol{m}'$ to the point under consideration. It decreases due to transitions leaving this point, i.e., we have the general relation

$$\dot{P}(\boldsymbol{m}, t) = \text{rate in} - \text{rate out}. \tag{4.108}$$

Since the "rate in" consists of all transitions from initial points $\boldsymbol{m}'$ to $\boldsymbol{m}$, it is composed of the sum over the initial points. Each term of it is given by the probability to find the particle at point $\boldsymbol{m}'$, multiplied by the transition probability per unit time to pass from $\boldsymbol{m}'$ to $\boldsymbol{m}$. Thus we obtain

$$\text{rate in} = \textstyle\sum_{\boldsymbol{m}'} w(\boldsymbol{m}, \boldsymbol{m}')P(\boldsymbol{m}', t). \tag{4.109}$$

In a similar way we find for the outgoing transitions the relation

$$\text{rate out} = P(\boldsymbol{m}, t)\cdot\textstyle\sum_{\boldsymbol{m}'} w(\boldsymbol{m}', \boldsymbol{m}). \tag{4.110}$$

Putting (4.109) and (4.110) into (4.108) we obtain

$$\dot{P}(\boldsymbol{m}, t) = \textstyle\sum_{\boldsymbol{m}'} w(\boldsymbol{m}, \boldsymbol{m}')P(\boldsymbol{m}', t) - P(\boldsymbol{m}, t)\sum_{\boldsymbol{m}'} w(\boldsymbol{m}', \boldsymbol{m}) \tag{4.111}$$

which is called the *master equation* (Fig. 4.5). The crux to derive a master equation is not so much writing down the expressions (4.109) and (4.110), which are rather obvious, but to determine the transition rates w explicitly. This can be done in two ways. Either we can write down the w's by means of plausibility arguments. This has been done in the example of Section 4.2. Further important examples will be given later, applied to chemistry and sociology. Another way, however, is to derive the w's from first principles where mainly quantum statistical methods have to be used.

Exercise on 4.5

Why has one to assume a Markov process to write down (4.109) and (4.110)?

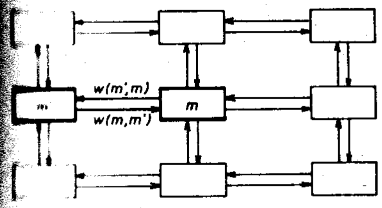

Fig. 4.5. Example of a network of the master equation

4.6 Exact Stationary Solution of the Master Equation for Systems in Detailed Balance

In this section we prove the following: If the master equation has a unique stationary solution ($\dot{P} = 0$) and fulfils the principle of detailed balance, this solution can be obtained explicitly by mere summations or, in the continuous case, by quadratures. The *principle of detailed balance* requires that there are as many transitions per second from state $\boldsymbol{m}$ to state $\boldsymbol{n}$ as from $\boldsymbol{n}$ to $\boldsymbol{m}$ by the inverse process. Or, in mathematical form:

$$w(\boldsymbol{n}, \boldsymbol{m})P(\boldsymbol{m}) = w(\boldsymbol{m}, \boldsymbol{n})P(\boldsymbol{n}). \tag{4.112}$$

In physics, the principle of detailed balance can be (in most cases) derived for systems in thermal equilibrium, using microreversibility. In physical systems far from thermal equilibrium or in nonphysical systems, it holds only in special case (for a counter example cf. exercise 1).

Equation (4.112) represents a set of homogeneous equations which can be solved only if certain conditions are fulfilled by the w's. Such conditions can be derived, for instance, by symmetry considerations or in the case that w can be replaced by differential operators. We are not concerned, however, with this question here, but want to show how (4.112) leads to an explicit solution. In the following we assume that $P(\boldsymbol{n}) \neq 0$. Then (4.112) can be written as

$$\frac{P(\boldsymbol{m})}{P(\boldsymbol{n})} = \frac{w(\boldsymbol{m}, \boldsymbol{n})}{w(\boldsymbol{n}, \boldsymbol{m})}. \tag{4.113}$$

Writing $\boldsymbol{m} = \boldsymbol{n}_{j+1}$, $\boldsymbol{n} = \boldsymbol{n}_j$, we pass from $\boldsymbol{n}_0$ to $\boldsymbol{n}_N$ by a chain of intermediate states. Because there exists a unique solution, at least one chain must exist. We then find

$$\frac{P(\boldsymbol{n}_N)}{P(\boldsymbol{n}_0)} = \textstyle\prod_{j=0}^{N-1} \dfrac{w(\boldsymbol{n}_{j+1}, \boldsymbol{n}_j)}{w(\boldsymbol{n}_j, \boldsymbol{n}_{j+1})}. \tag{4.114}$$

Putting

$$P(\boldsymbol{m}) = \mathcal{N} \exp \Phi(\boldsymbol{m}) \tag{4.115}$$

where $\mathcal{N}$ is the normalization factor, (4.114) may be written as

$$\Phi(\boldsymbol{n}_N) - \Phi(\boldsymbol{n}_0) = \sum_{j=0}^{N-1} \ln \{w(\boldsymbol{n}_{j+1}, \boldsymbol{n}_j)/w(\boldsymbol{n}_j, \boldsymbol{n}_{j+1})\}. \tag{4.116}$$

Because the solution was assumed to be unique, $\Phi(\boldsymbol{n}_N)$ is independent of the path chosen. Taking a suitable limit one may apply (4.116) to continuous variables.

As an *example* let us consider a linear chain with nearest neighbor transitions. Since detailed balance holds (cf. exercise 2) we may apply (4.114). Abbreviating transition probabilities by

Balance equation: flux is constant
But flux must ...
So flux = 0 ⇒ detailed balance.

$$w(m, m-1) = w_+(m) \tag{4.117}$$
$$w(m, m+1) = w_-(m) \tag{4.118}$$

we find

$$P(m) = P(0) \prod_{m'=0}^{m-1} \frac{w(m'+1, m')}{w(m', m'+1)} = P(0) \prod_{m'=0}^{m-1} \frac{w_+(m'+1)}{w_-(m')}. \tag{4.119}$$

In many practical applications, w_+ and w_- are "smooth" functions of m, since m is generally large compared to unity in the regions of interest. Plotting $P(m)$ gives then a smooth curve showing extrema (compare Fig. 4.6). We establish *conditions for extrema*. An extremum (or stationary value) occurs if

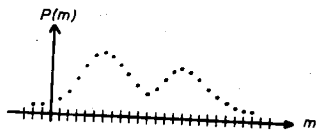

Fig. 4.6. Example of $P(m)$ showing maxima and minima

$$P(m_0) = P(m_0 + 1). \tag{4.120}$$

Since we obtain $P(m_0 + 1)$ from $P(m_0)$ by multiplying

$P(m_0)$ by $\dfrac{w_+(m_0+1)}{w_-(m_0)}$, exactly?

(4.120) implies $$\frac{w_+(m_0+1)}{w_-(m_0)} = 1. \tag{4.121}$$

$P(m_0)$ is a maximum, if

$$\left.\begin{array}{ll} P(m) < P(m_0) & \text{for } m < m_0 \\ \text{and for} & m > m_0 \end{array}\right\} \tag{4.122}$$

Equivalently, $P(m_0)$ is a maximum if (and only if)

$$\begin{aligned} &\frac{w_+(m+1)}{w_-(m)} > 1 \quad \text{for} \quad m < m_0, \\ &\frac{w_+(m+1)}{w_-(m)} < 1 \quad \text{for} \quad m > m_0. \end{aligned} \tag{4.123}$$

In both cases, (4.122) and (4.123), the numbers m belong to a finite surrounding of m_0.

Exercises on 4.6

1) Verify that the process depicted in Fig. 4.7 does not allow for detailed balance.

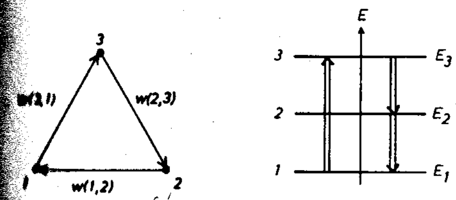

Fig. 4.7. Circular transitions violating the principle of detailed balance, e.g., in a three-level atom (right) $1 \to 3$: pump from external source, $3 \to 2$, $2 \to 1$ recombination of electron

2) Show: in a linear chain m with nearest neighbor transitions $m \to m \pm 1$ the principle of detailed balance always holds. Flux must be constant in equil.
3) What are the conditions that $P(m_0)$ is a minimum?
4) Generalize the extremal condition to several dimensions, i.e., $m \to \boldsymbol{m} = (m_1, m_2, \ldots, m_N)$, and nearest neighbor transitions.
5) Determine extrema and determine $P(m)$ explicitly for

a) $w(m, m \pm 1) = w,$
$w(m, m + n) = 0, n \neq \pm 1$

Note: normalize P only in a finite region $-M \leq m \leq M$, and put $P(m) = 0$ otherwise. but this will ruin Equilibrium

b) $w(m, m+1) = \dfrac{m+1}{N} w_0 \quad \text{for} \quad 0 \leq m \leq N-1$

$w(m, m-1) = \dfrac{N-m+1}{N} w_0 \quad \text{for} \quad 1 \leq m \leq N$

$w(m, m') = 0$ otherwise.

c) $w(m+1, m) = w_+(m+1) = \alpha(m+2) \quad m \geq 0$
$w(m, m+1) = w_-(m) = \beta(m+1)(m+2).$

Including this constant flux q in calculation of $\vec{\pi}$
$q = 0$ by uniqueness of $\vec{\pi}$ if transition rates decay rapidly enough. If no solution exists for $q = 0$ because of nonnormalizability, introduction of $q \neq 0$ can only cure divergence at one end and will create a positive divergence of $\Sigma \pi$ in other direction

Show that $P(m)$ is the Poisson distribution $\pi_{k,\mu}(\equiv a_k)$ (2.57) with $m \leftrightarrow k$ and $\mu \leftrightarrow \alpha/\beta$.
Hint: Determine $P(0)$ by means of the normalization condition

$$\sum_{m=0}^{\infty} P(m) = 1$$

d) Plot $P(m)$ in the cases a) – c).

4.7* The Master Equation with Detailed Balance. Symmetrization, Eigenvalues and Eigenstates

We write the master equation (4.111) in the form

$$\sum_n L_{mn} P(n) = \dot{P}(m) \tag{4.124}$$

where we have used the abbreviation

$$L_{m,n} = w(m, n) - \delta_{m,n} \sum_l w(l, n). \tag{4.125}$$

The master equation represents a set of linear differential equations of first order. To transform this equation into an ordinary algebraic equation we put

$$P(m) = \mathrm{e}^{-\lambda t} \varphi_m \tag{4.126}$$

where φ_m is time independent. Inserting (4.126) into (4.124) yields

$$\sum_n L_{mn} \varphi_n^{(\alpha)} = -\lambda_\alpha \varphi_m^{(\alpha)}. \tag{4.127}$$

The additional index α arises because these algebraic equations allow for a set of eigenvalues λ and eigenstates φ_n which we distinguish by an index α. Since in general the matrix L_{mn} is not symmetric the eigenvectors of the adjoint problem

$$\sum_m \chi_m^{(\alpha)} L_{mn} = -\lambda_\alpha \chi_n^{(\alpha)} \tag{4.128}$$

are different from the eigenvectors of (4.127). However, according to well-known results of linear algebra, φ and χ form a biorthonormal set so that

$$(\chi^{(\alpha)}, \varphi^{(\beta)}) \equiv \sum_n \chi_n^{(\alpha)} \varphi_n^{(\beta)} = \delta_{\alpha,\beta}. \tag{4.129}$$

In (4.129) the lhs is an abbreviation for the sum over n. With help of the eigenvectors φ and χ, L_{mn} can be written in the form

$$L_{mn} = -\sum_\alpha \lambda_\alpha \varphi_m^{(\alpha)} \chi_n^{(\alpha)}. \tag{4.130}$$

→ but this assumes completeness

We now show that the matrix occurring in (4.127) can be symmetrized. We first

might be ok for detailed balance since symmetrizable

define the symmetrized matrix by

$$L^s_{m,n} = w(m, n) \frac{P^{1/2}(n)}{P^{1/2}(m)} \tag{4.131}$$

for $m \neq n$. For $m = n$ we adopt the original form (4.125). $P(n)$ is the stationary solution of the master equation. It is assumed that the detailed balance condition

$$w(m, n) P(n) = w(n, m) P(m) \tag{4.132}$$

holds. To prove that (4.131) represents a symmetric matrix, $\mathbf{L}^s$, we exchange in (4.131) the indices n, m

$$L^s_{n,m} = w(n, m) \frac{P^{1/2}(m)}{P^{1/2}(n)}. \tag{4.133}$$

By use of (4.132) we find

$$(4.133) = w(m, n) \frac{P(n)}{P(m)} \cdot \frac{P^{1/2}(m)}{P^{1/2}(n)} \tag{4.134}$$

which immediately yields

$$L^s_{m,n} \tag{4.135}$$

so that the symmetry is proven. To show what this symmetrization means for (4.127), we put

$$\varphi_n^{(\alpha)} = P_{(n)}^{1/2} \tilde{\varphi}_n^{(\alpha)} \tag{4.136}$$

which yields

$$\sum_n L_{mn} P_{(n)}^{1/2} \tilde{\varphi}_n^{(\alpha)} = -\lambda_\alpha P_{(m)}^{1/2} \tilde{\varphi}_m^{(\alpha)}. \tag{4.137}$$

Dividing this equation by $P_{(m)}^{1/2}$ we find the symmetrized equation

$$\sum_n L^s_{mn} \cdot \tilde{\varphi}_n^{(\alpha)} = -\lambda_\alpha \tilde{\varphi}_m^{(\alpha)}. \tag{4.138}$$

We proceed with (4.128) in an analogous manner. We put

$$\chi_n^{(\alpha)} = P_{(n)}^{-1/2} \tilde{\chi}_n^{(\alpha)}, \tag{4.139}$$

insert it into (4.128) and multiply by $P^{1/2}(n)$ which yields

$$\sum_m \tilde{\chi}_m^{(\alpha)} L^s_{mn} = -\lambda_\alpha \tilde{\chi}_n^{(\alpha)}. \tag{4.140}$$

The $\tilde{\chi}$'s may be now identified with the $\tilde{\varphi}$'s because the matrix L^s_{mn} is symmetric.

This fact together with (4.136) and (4.139) yields the relation

$$\varphi_n^{(\alpha)} = P(n)\chi_n^{(\alpha)}. \tag{4.141}$$

Because the matrix L^s is symmetric, the eigenvalues λ can be determined by the following variational principles as can be shown by a well-known theorem of linear algebra. The following expression must be an extremum:

$$-\lambda = \text{Extr.}\left\{\frac{(\tilde{\chi}L^s\tilde{\chi})}{(\tilde{\chi}\tilde{\chi})}\right\} = \text{Extr.}\left\{\frac{(\chi L\varphi)}{(\chi\varphi)}\right\}. \tag{4.142}$$

balance condition

$\tilde{\chi}_n$ has to be chosen so that it is orthogonal to all lower eigenfunctions. Furthermore, one immediately establishes that if we chose $\chi_n^{(0)} = 1$, then on account of

$\Rightarrow \tilde{\chi}_n^{(0)} = P(n)^{1/2}$

$$\textstyle\sum_m L_{m,n} = 0 \tag{4.143}$$

the eigenvalue $\lambda = 0$ associated with the stationary solution results. We now show that all eigenvalues λ are nonnegative. To this end we derive the numerator in (4.142)

$$\textstyle\sum_{m,n} \chi_m L_{m,n} P(n)\chi_n \tag{4.144}$$

(compare (4.139), (4.141), and (4.131)) in a way which demonstrates that this expression is nonpositive. We multiply $w(m, n)P(n) \geq 0$ by $-1/2(\chi_m - \chi_n)^2 \leq 0$ so that we obtain

No, not quite true since φ and χ are linked by (4.141)

$$-\textstyle\sum_{m,n} \frac{1}{2}(\chi_m - \chi_n)^2 w(m, n)P(n) \leq 0. \tag{4.145}$$

The evaluation of the square bracket yields

$$\underset{(1)}{-\tfrac{1}{2}\textstyle\sum_{m,n} \chi_m^2 w(m, n)P(n)} \; \underset{(2)}{- \tfrac{1}{2}\textstyle\sum_{m,n} \chi_n^2 w(m, n)P(n)} \; \underset{(3)}{+ \textstyle\sum_{m,n} \chi_m\chi_n w(m, n)P(n)}. \tag{4.146}$$

In the second sum we exchange the indices m, n and apply the condition of detailed balance (4.132). We then find that the second sum equals the first sum, thus that (4.146) agrees with (4.144). Thus the variational principle (4.142) can be given the form

$$\lambda = \text{Extr}\left\{\frac{\frac{1}{2}\sum_{m,n} (\chi_m - \chi_n)^2 w(m, n)P(n)}{\sum_n \chi_n^2 P(n)}\right\} \geq 0! \tag{4.147}$$

from which it is evident that λ is nonnegative. Furthermore, it is evident that if we chose χ = const., we obtain the eigenvalue $\lambda = 0$.

4.8* Kirchhoff's Method of Solution of the Master Equation

We first present a simple counter example to the principle of detailed balance. Consider a system with three states 1, 2, 3, between which only transition rates $w(1, 2)$, $w(2, 3)$ and $w(3, 1)$ are nonvanishing. (Such an example is provided by a three-level atom which is pumped from its first level to its third level, from where it decays to the second, and subsequently to the first level, cf. Fig. 4.7). On physical grounds it is obvious that $P(1)$ and $P(2) \neq 0$ but due to $w(2, 1) = 0$, the equation

$$w(2, 1)P(1) = w(1, 2)P(2) \tag{4.148}$$

required by detailed balance cannot be fulfilled. Thus other methods for a solution of the master equation are necessary. We confine our treatment to the stationary solution in which case the master equation, (4.111), reduces to a linear algebraic equation. One method of solution is provided by the methods of linear algebra. However, that is a rather tedious procedure and does not use the properties inherent in the special form of the master equation. We rather present a more elegant method developed by Kirchhoff, originally for electrical networks. To find the stationary solution $P(n)$ of the master equation[2],

$$\textstyle\sum_{n=1}^{N} w(m, n)P(n) - P(m)\sum_{n=1}^{N} w(n, m) = 0, \tag{4.149}$$

and subject to the normalization condition

$$\textstyle\sum_{n=1}^{N} P(n) = 1 \tag{4.150}$$

we use a little bit of graph theory.

We define a graph (or, in other words a figure) which is associated with (4.149). This graph G contains all vertices and edges for which $w(m, n) \neq 0$. Examples of graphs with three or four vertices are provided by Fig. 4.8. For the following solution, we must consider certain parts of the graph G which are obtained from G by omitting certain edges. This subgraph, called maximal tree $T(G)$, is defined as follows:

1) $T(G)$ covers subgraph so that
   a) all edges of $T(G)$ are edges of G,
   b) $T(G)$ contains all vertices of G.
2) $T(G)$ is connected.
3) $T(G)$ contains no circuits (cyclic sequence of edges).

This definition, which seems rather abstract, can best be understood by looking at examples. The reader will immediately realize that one has to drop a certain minimum number of edges of G. (Compare Figs. 4.9 and 4.10). Thus in order to

[2] When we use n instead of the vector, this is not a restriction because one may always rearrange a *discrete* set in the form of a sequence of single numbers.

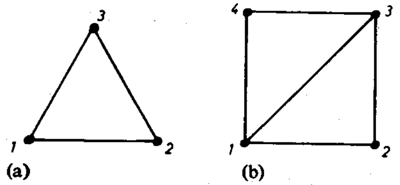

Fig. 4.8a and b. Examples of graphs with 3 or 4 vertices

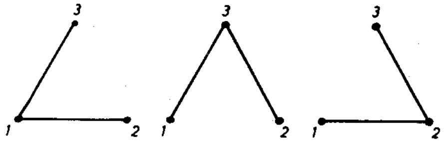

Fig. 4.9. The maximal trees $T(G)$ belonging to the graph of Fig. 4.8a

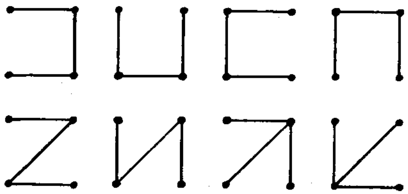

Fig. 4.10. The maximal trees $T(G)$ belonging to the graph G of Fig. 4.8b

obtain the maximal trees of Fig. 4.8b one has to drop in Fig. 4.8b either one side *and* the diagonal or two sides.

We now define a directed maximal tree with index n, $T_n(G)$. It is obtained from $T(G)$ by directing all edges of $T(G)$ towards the vertex with index n. The directed maximal trees belonging to $n = 1$, Fig. 4.9, are then given by Fig. 4.11. After these preliminaries we can give a recipe how to construct the stationary solution $P(n)$. To this end we ascribe to each directed maximal tree a numerical value called A: A $(T_n(G))$: This value is obtained as product of all transition rates $w(n, m)$ whose edges occur in $T_n(G)$ in the corresponding direction. In the example of Fig. 4.11 we thus obtain the following different directed maximal trees

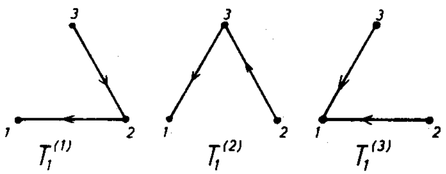

Fig. 4.11. The directed maximal trees T_1 belonging to Fig. 4.9 and $n = 1$

$$T_1^{(1)}: w(1, 2)w(2, 3) = A(T_1^{(1)}) \tag{4.151}$$

$$T_1^{(2)}: w(1, 3)w(3, 2) = A(T_1^{(2)}) \tag{4.152}$$

$$T_1^{(3)}: w(1, 2)w(1, 3) = A(T_1^{(3)}) \tag{4.153}$$

(It is best to read all arguments from right to left). Note that in our example Fig. 4.11 $w(3, 2) = w(1, 3) = 0$. We now come to the last step. We define S_n as the sum over all maximal directed trees with the same index n, i.e.,

$$S_n = \sum_{\text{all } T_n(G)} A(T_n(G)). \tag{4.154}$$

In our triangle example we would have, for instance,

$$\begin{aligned} S_1 &= w(1, 2)w(2, 3) + w(1, 3)w(3, 2) + w(1, 2)w(1, 3) \\ &= w(1, 2)w(2, 3) \quad (\text{since } w(3, 2) = w(1, 3) = 0). \end{aligned} \tag{4.155}$$

Kirchhoff's formula for the probability distribution P_n is then given by

$$P_n = \frac{S_n}{\sum_{l=1}^{N} S_l}. \tag{4.156}$$

In our standard example we obtain using (4.151) etc.

$$P_1 = \frac{w(1, 2)w(2, 3)}{w(1, 2)w(2, 3) + w(2, 3)w(3, 1) + w(3, 1)w(1, 2)}. \tag{4.157}$$

Though for higher numbers of vertices this procedure becomes rather tedious, at least in many practical cases it allows for a much deeper insight into the construction of the solution. Furthermore it permits decomposing the problem into several parts for example if the master equation contains some closed circles which are only connected by a single line.

Exercise on 4.8

Consider a chain which allows only for nearest neighbor transitions. Show that Kirchhoff's formula yields exactly the formula (4.119) for detailed balance.

4.9* Theorems about Solutions of the Master Equation

We present several theorems which are important for applications of the master equation. Since the proofs are purely mathematical, without giving us a deeper insight into the processes, we drop them. We assume the w's are *independent* of time.

1) There exists always at least one stationary solution $P(m)$, $\dot{P}(m) = 0$.
2) This stationary solution is unique, provided the graph G of the master equation is connected (i.e., any two pairs of points m, n can be connected by at least one sequence of lines (over other points)). (irreducible)
3) If at an initial time, $t = 0$,

$$0 \le P(m, 0) \le 1 \tag{4.158}$$