EXPANSION OF THE MASTER EQUATION FOR
A BIOMOLECULAR SELECTION MODEL

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A stochastic model based on Eigen and Schuster's theory of biomolecular self-replication is studied by treating the master equation with the system-size expansion technique. The steady-state results are found to be in good agreement with the previous results and with those derived from the principle of detailed balancing. Multispecies competition and co-existence are studied carefully with the conclusions that a stable steady state is predicted for the former and a metastable state for the latter. The stochastic selection processes are also analyzed and discussed.

1. Introduction. Recently, Eigen and Schuster's theory of biomolecular self-replication (Eigen, 1971; Eigen and Schuster, 1979) was studied stochastically (Jones and Leung, 1981; Leung, 1984). Owing to the nonlinear nature of the model, the corresponding master equation is practically unsolvable. Even the moment equations have to be truncated so that the average molecular numbers and the variances can be studied approximately. Most stochastic behaviors are indeed included in the first two moments, however, it would be more desirable to evaluate the probability distribution function from which more stochastic aspects of the self-replication processes will be revealed. An alternate approximation is needed to achieve this goal. We note also that the moment-expansion scheme (Jones and Leung, 1981) involves the neglect of the third correlation. This and higher-order correlations have been recently found to be important, for some cases, even in the linear system (Schuster and Sigmund, private communication). In this paper, results from different approximation schemes will be compared.

The model system under consideration consists of \( N \) species of biomolecular information carriers which are capable of replicating themselves accurately. External constraint is imposed so that the carrying capacity of the system is \( \Omega \), while the total number of molecules in the system is variable. The deterministic equations describing the self-replication processes are given by,

\[
dn_i/dt = g(n_i) - r_i(n),
\]

with

\[
g(n_i) = A_i n_i, \quad r_i(n) = D_i n_i + \sum_j W_{ij} n_j n_i / \Omega.
\]
In the above, \( n_i \) is the number of molecules for the \( i \)th species and \( W_i = A_i - D_i \) is the selective value. \( A_i \) and \( D_i \) are respectively the self-replication and the degradation rates.

In equation (1), the complicated processes of molecular replication are treated as the single-step autocatalytic reaction, so that the master equation approach developed for chemical dynamics (McQuarrie, 1967) can then be employed to describe the stochastic behaviors of the model system. The probability of having \( n_j \) molecules of species \( j \) at the time \( t \) is described by the probability function \( P((n); t) \) which satisfies the master equation (Gardiner, 1983),

\[
\frac{\partial P((n); t)}{\partial t} = \sum_j (g(n_j - 1)P(n_1 \ldots n_j - 1 \ldots n_N; t) + r_j(n_1 \ldots n_j + 1 \ldots n_N)P(n_1 \ldots n_j + 1 \ldots n_N; t) - [g(n_j) + r_j((n))]P((n); t)).
\]

This stochastic description is valid for a system with large \( \Omega \) since a correct stochastic theory must reduce to the deterministic formulation in the thermodynamic limit of \( \Omega \to \infty \) (Oppenheim et al., 1969; Kurtz, 1972). We have shown previously, with the moment expansion approximation scheme, that this master equation (3) produces approximately the deterministic rate equation together with fluctuations which are insignificant if \( \Omega \) is large (Jones and Leung, 1981; Leung, 1984). These facts also enable us to employ the system-size expansion approximation (Van Kampen, 1976; Van Kampen, 1981) to expand the master equation (3). This new treatment allows the determination of the otherwise mathematically inaccessible but biologically interesting regime, and provides new results which can be used to compare with those derived from a different approximation scheme.

2. Expansion of the Master Equation. The system-size expansion technique was designed to treat the stochastic problems with small relative fluctuations (Van Kampen, 1976). Each variable \( n_j(t) \) can be split into deterministic and stochastic parts,

\[
n_j(t) = \Omega \phi_j(t) + \Omega^{1/2} x_j(t).
\]

The probability function \( P((n); t) \) now goes over to \( \Pi((x); t) \) which describes the probability of having the fluctuating component \( x_j(t) \) while its deterministic part is \( \phi_j(t) \). These two probability functions are related by,

\[
\Pi((x); t) = \Omega^{1/2} P((n); t).
\]

After substitution and expansion, equation (3) reduces to