Collective Excitations in Low Dimensional Systems and Stochastic Control of Population Growth in A Fluctuating Environment

by

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Abstract

In this thesis, I study several problems in the following areas: collective excitations in condensed matter physics, noise in gene network and stochastic control in biophysics. In the first area, I construct an effective field theory to describe Bose-Einstein Condensate (BEC) realized in an external potential. This theory explicitly explores the idea of spontaneous symmetry breaking and its application in the description of phase transitions of confined systems. Based on the effective lagrangian, I calculate the excitation spectrum and Matsubara Green's functions using the method of functional integrals. The theory also shows that in one dimension the collective excitation of a bosonic system can be unified with that of a fermionic system, which is described by Luttinger liquid theory. The unified theory of collective excitations of low dimensional quantum systems motivates my study of collective excitations of interacting classical particles confined in one dimension. It is shown in my paper that the structure of Hamiltonian or Lagrangian for one dimensional constrained systems is uniquely determined by conservation laws. Therefore the excitations of bosonic, fermionic and classical particles are strikingly similar in one dimension. In the second area, i. e., noise in gene networks and phenotypic switching in a fluctuating environment, I study the noise propagation in a gene network cascade using the method of master equations which examines the validity of the more popular methods such as the Langevin equation. To further explore the applications of stochastic processes for complex systems, I study phenotypic switches in a fluctuating environment. By combining the techniques of stochastic differential equation and stochastic dynamical programming, I propose a simple framework which can be used to study phenotypic growth dynamics. Another work is to explore the influence of environment on the dynamical properties of small systems is directed to the unusual blinking statistics of semiconductor quantum dots. I show in a model system that a broad spectrum of decay rates is possible when disorder is present in the environment.

Thesis Supervisor: Robert J. Silbey

Title: Dean of Science and Class of '42 Professor of Chemistry

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At the time I am about to finish this Ph.D. thesis, I find the most difficult part is the Acknowledgements. A physical picture can be drawn nicely in several equations; the equations can be displayed beautifully using the magic of Latex; however, it is far beyond the abilities of any of these to express my gratitude to so many people. In this sense, my acknowledgements are incomplete. The guidance that I have received, the friendship that I have developed and so many memorable moments will persist. Never forget.

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Chapter 1

Effective Quantum Field Theory for Bose Einstein Condensate

Ordinary phase transitions occur at a true macroscopic level; however, quantum phase transitions are are much more difficult at this level. Experimental realization of these types of phase transitions are usually achieved in extreme conditions: high magnetic/electric field, extremely low temperature and state of art nano-fabrication, which are all aimed at achieving geometric confinement. From the theoretical point of view, a confined geometry is necessary since the mean energy spacing is inversely proportional to the size of the system. Therefore one of the solutions to reduce thermal effects is to set up an artificial confining potential. This also brings challenges to theorists as most of the standard phase transition theories and quantum many-body theories assume an infinitely large system and no spacial confinement. Even though certain symmetries are not available at the onset, new constraints, nevertheless, show up. In addition, the nature of phase transitions is not changed by confining potentials because it only relies on those symmetries that are spontaneously broken. These in fact are some of the keys that lead to successful theories. In this chapter we focus on one type of confined phase transitions, namely, Bose-Einstein Condensation (BEC) realized experimentally since 1995. We adopt an effective-field-theory view to describe the low-energy excitations of trapped Bose gases, which allows a direct and systematic way to investigate the consequences of spontaneous symmetry breaking. The derivation of the effective Lagrangian can incorporate various approximations and can reproduce the results obtained by the standard hydrodynamic approach. Based on the effective Lagrangian, we calculate the energy spectrum and Matsubara Green's function of trapped 1D Bose gases with $\delta-$function repulsive interaction, allowing the comparison of various results obtained by different approaches. We also analytically calculate the finite-temperature correlation function of trapped 2D Bose gases. The calculation scheme can be easily extended to higher dimensions. We find that particle interactions will always decrease the coherence length of the condensate in 2D, confirming recent numerical results. The validation of various asymptotic expressions are given.

1.1 Introduction

The problem of theoretically describing interacting Bose gases at low temperatures has a long history. Unlike fermionic problems, where by particle-hole transformation Wick's theorem can be applied, conventional perturbation theory can not be applied to bosons since neither creation nor annihilation operators annihilate the ground state, and as a result the application of Wick's theorem becomes much more complicated. The successful perturbative approach of Bogoliubov [1] is based on the observation of vanishing commutator in the thermodynamical limit ($N \to \infty, V \to \infty, N/V \to$ constant) and separating the creation and annihilation operators of the ground state into a $c-$number part and an operator correction part, which is assumed to be small. Bogoliubov's perturbation theory provides the basis for the modern theoretical treatment of the Bose-Einstein condensation(BEC) in a confining external potential, which was experimentally realized in 1995 [2].

The standard starting point of the modern treatment for nonuniform Bose gases at low temperatures is the Gross-Pitaevskii (GP) equation [3]:

$$i\hbar\partial_t\Psi(\mathbf{r},t) = \left(-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{ext}}(\mathbf{r}) + g|\Psi(\mathbf{r},t)|^2\right)\Psi(\mathbf{r},t) \tag{1.1}$$

where $\Psi(\mathbf{r},t)$ is the order parameter or wave function of the condensate, $V_{\text{ext}}(\mathbf{r})$ is the confining potential and the coupling constant g is related to the $s-$wave scattering length a by:

$$g = \frac{4\pi\hbar^2 a}{m} \tag{1.2}$$

The GP equation can be interpreted as a self-consistent Hartree equation for the condensate wave function, so it does not include the effect of the interaction with noncondensate atoms. In order to study low energy collective excitations, Stringari[4] developed a hydrodynamic approach, in which the GP equation is linearized in terms of density and phase fields. The collective excitations are sound waves with a modified dispersion law caused by the confining potentials. The hydrodynamic approach was further developed by Griffin *et al.*[5] where the classical density and phase fields are quantized and the sound waves become phonons. The hydrodynamic approach was applied extensively to study the excitation spectrum and phase coherence of Bose gases in deformed traps at $T \approx 0$ [6, 7, 8]. It was found that confining potentials play such an important role in suppressing quantum and thermal fluctuations that dispersion laws become discrete and there exists non-exponential decay of off-diagonal long range order, which indicates possible BEC at finite T in 2D and 1D. Numerical study [9, 10, 11] of collective excitations of BEC at finite temperatures were implemented by the finite-temperature Hartree-Fock-Bogoliubov(HFB) method. It was shown that the excitation frequencies have a weak temperature dependence while the condensate fraction is strongly depleted. Numerical calculations indicate disagreement of theoretical and experimental results at finite temperatures, so it would be desirable to obtain the Matsubara Green's functions for trapped gases analytically and give explicitly the validity conditions for various asymptotic expressions.

The hydrodynamic approach based on the GP equation, although powerful and efficient, may not be the most natural method for discussing the finite temperature behavior of interacting Bose gases. It is known that field-theoretical quantities such as the Green's function and vertex function can be expressed directly as functional averages. Furthermore, it is an advantage to study low energy physics in effective field theories facilitated by the functional method, see eg. Ref.[11] for a recent review. The functional approach to superfluids was developed by Popov [13], where the infrared-singularity difficulty encountered in conventional perturbation technique was alleviated by the method of successive integration over fast modes. One essentially obtained an effective field theory in terms of renormalized coupling constants and slow modes. This approach was further developed by Bogoliubov *et al.* [14, 15, 16] to study BEC in confined potentials. A slightly different way to obtain the effective Lagrangian was adopted in [17, 18, 19], where a polar coordinate transformation was performed first. In this paper, we view BEC as a result of spontaneous breaking of global $U(1)$ symmetry and derive an effective Lagrangian of the corresponding Nambu-Goldstone bosons for the general cases of trapped Bose gases. Despite the recent developments of techniques for calculating correlation functions in BEC, the confining potential makes the problem quite complicated so that one must resort to approximations and regulations in order to obtain simple asymptotic behavior, which leads to different results, e.g. for condensate density [7, 16], exponents of the 1D equal-time single particle correlation function power law etc. So it is important to compare and unify the results obtained by hydrodynamic and functional approaches.

1.2 Effective Lagrangian Approach

1.2.1 Derivation of Effective Lagrangian

Let us consider a weakly interacting Bose gas confined in an external potential $V_{\text{ext}}(\mathbf{r})$ in $D+1$ dimensions. The partition function can be written as:

$$Z[\psi^*, \psi] = \int \mathcal{D}\psi^* \mathcal{D}\psi \; e^{-\int_0^\beta d\tau \int d^D r \mathcal{L}} \tag{1.3}$$

where the Euclidean Lagrangian $\mathcal{L}$ is

$$\mathcal{L} = \psi^* \partial_\tau \psi + \frac{\hbar^2}{2m} \nabla\psi^* \nabla\psi + [V_{\text{ext}}(\mathbf{r}) - \mu]\psi^*\psi + \frac{g_D}{2}(\psi^*\psi)^2 \tag{1.4}$$

The bosons interact with $\delta-$function repulsion and g_D is the coupling constant. Here $\beta = \frac{1}{k_B T}$ and μ is chemical potential. It is clear that the Euler-Lagrange equation of motion for the field ψ^* yields the GP equation (1.1) with $\tau \to it/\hbar$. To facilitate the analysis of spontaneous symmetry breaking, it is useful to absorb the third term in (1.4) into the interaction term to obtain:

$$\mathcal{L} = \psi^* \partial_\tau \psi + \frac{\hbar^2}{2m} \nabla \psi^* \nabla \psi + V(\psi^* \psi) \tag{1.5}$$

and

$$V(\psi^* \psi) = \frac{g_D}{2} (\psi^* \psi - \rho_0(\mathbf{r}))^2 \tag{1.6}$$

is a field potential, of which $\rho_0(\mathbf{r})$ is the potential minimum:

$$\rho_0(\mathbf{r}) = \frac{1}{g_D} [\mu - V_{\text{ext}}(\mathbf{r})] \tag{1.7}$$

It is clear $\mathcal{L}$ is invariant under a global $U(1)$ symmetry transformation:

$$\psi \to e^{i\theta} \psi \tag{1.8}$$

The Goldstone theorem predicts the existence of massless bosons when the global $U(1)$ symmetry is spontaneously broken. Since we wish to construct an effective Lagrangian for low-energy processes, the Nambu-Goldstone boson field must appear in the effective Lagrangian. It is well-known that the Nambu-Goldstone boson is completely decoupled in the limit of vanishing momentum. This implies that, by a proper transformation of field variables, the Nambu-Goldstone bosonic field should drop out of field potential term, $V(\psi^* \psi)$, and this naturally suggests the following choice for field variables:

$$\psi(\mathbf{r}, \tau) = \sqrt{\rho(\mathbf{r}, \tau)} e^{i\theta(\mathbf{r}, \tau)} \tag{1.9a}$$

$$\psi^*(\mathbf{r}, \tau) = \sqrt{\rho(\mathbf{r}, \tau)} e^{-i\theta(\mathbf{r}, \tau)} \tag{1.9b}$$

Under the transformation (1.8), θ transforms as: $\theta \longrightarrow \theta+\alpha$, where α is a constant. Since $\mathcal{L}$ is invariant under this transformation, the effective lagrangian $\mathcal{L}_{\text{eff}}$ must contain θ in derivative forms to preserve the symmetry. A general form of $\mathcal{L}_{\text{eff}}$ can then be written as:

$$\mathcal{L}_{\text{eff}} = \frac{1}{2} g_{\mu\nu} \partial_\mu \theta \partial_\nu \theta + h.d.t. \tag{1.10}$$

where $g_{\mu\nu}$ can be interpreted as an Euclidean metric tensor. For an inhomogeneous situation $g_{\mu\nu}$ can be different from a constant metric. $h.d.t.$ denotes terms in higher powers of $\partial_\mu\theta$ and coupling terms of $\partial_\mu\theta$ with other degrees of freedom. In the low energy regime, by power counting, only the first or the first few terms in (1.10) are needed. Working with the effective Lagrangian, $\mathcal{L}_{\text{eff}}$, should allow easier calculations and give same results as those obtained by original Lagrangian $\mathcal{L}$.

Now we will perform the matching process as the following: By appropriate scaling, i.e. $\psi \longrightarrow \frac{\psi}{\sqrt{g_D}}$, one finds $\mathcal{L} \longrightarrow \frac{\mathcal{L}}{g_D}$. So g_D plays the role of $\hbar$, when g_D is small, and we can use the semiclassical approximation, namely setting all derivatives to zero and minimizing the field potential energy, to obtain the Thomas-Fermi ground state configuration:

$$\begin{aligned} \rho_{TF}(\mathbf{r}) &= \rho_0(\mathbf{r})\vartheta\left(\rho_0(\mathbf{r})\right) \\ &= \frac{1}{g_D}[\mu - V_{\text{ext}}(\mathbf{r})]\vartheta\left(\mu - V_{\text{ext}}(\mathbf{r})\right) \end{aligned} \tag{1.11}$$

where $\vartheta(x)$ is the step function. The ground state configuration (1.11) is valid provided that physical bosons are weakly interacting. The condensate density, $\rho_{TF}(\mathbf{r})$, can also be obtained from the GP equation using the TFA. By choosing this nonzero ground state configuration the global $U(1)$ symmetry is spontaneously broken. Define the dynamic density:

$$\begin{aligned} \rho(\mathbf{r},\tau) &\equiv \psi^*(\mathbf{r},\tau)\psi(\mathbf{r},\tau) \\ &= \rho_{TF}(\mathbf{r}) + \sigma(\mathbf{r},\tau) \end{aligned} \tag{1.12}$$

which can be decomposed into a static part $\rho_{TF}(\mathbf{r})$ and a fluctuating part $\sigma(\mathbf{r},\tau)$. The fluctuating density $\sigma(\mathbf{r}, \tau)$ generally includes contributions from thermal and quantum fluctuations of the condensate and the non-condensate. At low temperatures, we expect

$$\rho_{TF}(\mathbf{r}) \gg \sigma(\mathbf{r}, \tau) \tag{1.13}$$

In terms of $\rho(\mathbf{r}, \tau)$ and $\theta(\mathbf{r}, \tau)$, the Lagrangian becomes:

$$\mathcal{L} = \frac{1}{2}\partial_\tau \rho + i\rho\partial_\tau\theta + \frac{\hbar^2}{2m}\left[\frac{1}{4\rho}\left(\nabla\rho\right)^2 + \rho\left(\nabla\theta\right)^2\right] + \frac{1}{2}g_D(\rho - \rho_0)^2 \tag{1.14}$$

The first term is a total derivative and can be dropped. In the low energy regime, (1.13) holds and we can expand (1.14) in powers of $\frac{\sigma}{\rho_{TF}}$ using (1.12):

$$\begin{aligned} \mathcal{L} = \quad & i\rho_{TF}\partial_\tau\theta + \frac{\hbar^2}{2m}\rho_{TF}(\nabla\theta)^2 \\ & + \frac{\hbar^2}{2m}\left[\frac{1}{2}\nabla\ln\rho_{TF}\cdot\nabla\sigma - \frac{1}{4}(\nabla\ln\rho_{TF})^2\sigma + (\nabla\theta)^2\sigma\right] - g_D\rho_0\sigma\vartheta(-\rho_0) + i(\partial_\tau\theta)\sigma \\ & + \left[\frac{1}{2}g_D + \frac{\hbar^2}{8m\rho_{TF}}(\nabla\ln\rho_{TF})^2\right]\sigma^2 + \frac{\hbar^2}{8m\rho_{TF}}(\nabla\sigma)^2 - \frac{\hbar^2}{4m\rho_{TF}}\sigma\nabla\ln\rho_{TF}\cdot\nabla\sigma \\ & + O\left(\left(\frac{\sigma}{\rho_{TF}}\right)^3\right) \end{aligned} \tag{1.15}$$

The first line describes the dynamics of the phase field $\theta(\mathbf{r}, \tau)$. The second and third lines are coupling of fluctuating density field $\sigma(\mathbf{r}, \tau)$ with the static condensate and the phase field (phonon excitations) in linear and quadratic orders of $\frac{\sigma}{\rho_{TF}}$. For low-energy processes, it is sufficient to truncate the series at the quadratic level and the contribution from σ field can be easily evaluated. On the other hand, if one is interested in noncondensate dynamics, the $\theta(\mathbf{r}, \tau)$ field should be integrated out instead for the effective Lagrangian. Now by integrating over the σ field, we arrive at:

$$\begin{aligned}\mathcal{L} = \; & \left[i\partial_\tau\theta + \frac{\hbar^2}{2m}(\nabla\theta)^2 - \frac{\hbar^2}{8m}\left(2\nabla^2\ln\rho_{TF} + (\nabla\ln\rho_{TF})^2\right)\right] \\ & \times \frac{1}{\frac{\hbar^2}{2m\rho_{TF}}\left[\nabla^2 + 2\nabla\ln\rho_{TF}\cdot\nabla - (\nabla\ln\rho_{TF})^2\right] - 2g_D} \\ & \times \left[i\partial_\tau\theta + \frac{\hbar^2}{2m}(\nabla\theta)^2 - \frac{\hbar^2}{8m}\left(2\nabla^2\ln\rho_{TF} + (\nabla\ln\rho_{TF})^2\right)\right] + \frac{\hbar^2}{2m}\rho_{TF}(\nabla\theta)^2\end{aligned} \tag{1.16}$$

where we dropped the term $i\rho_{TF}\partial_\tau\theta$, which essentially imposes the conservation of ρ_{TF}. The following scaling analysis will help to simplify (1.16): ∇^2, $2\nabla\ln\rho_{TF}\cdot\nabla$ and $(\nabla\ln\rho_{TF})^2$ scale as R^{-2} and they should become negligible to $2g_D$ at large distances. We can define a length scale ξ such that:

$$\frac{\hbar^2}{2m\rho_{TF}}\cdot\frac{2}{\xi^2} = 2g_D$$

i.e.

$$\xi(\mathbf{r}) = \frac{\hbar}{\sqrt{2m\rho_{TF}(\mathbf{r})g_D}} \tag{1.17}$$

above which we can safely neglect the gradient terms in the demonimator of (1.16). We see that $\xi(\mathbf{r})$ defined above is just the healing length and it is a spatially dependent quantity due to the confining potentials. $\xi(\mathbf{r})$ is larger near the edge than in the center of a trap. The approximation we made here is often called TFA, originally proposed to calculate the electron density and potential energy of atoms self-consistently[20]. It is useful to estimate the ratio of healing length ξ to the average inter-particle distance d in 3D: $d = (\frac{1}{\bar{\rho}})^{1/3}$. Given the coupling constant g_3 in (1.2), $\frac{\xi}{d} \sim (\bar{\rho}a^3)^{-1/6}$. Typical values of Bose gas density in experiments range from $10^{13} \sim 10^{15}\text{cm}^{-3}$, while the scattering length $a \sim 10^{-7}\text{cm}$, so $\frac{\xi}{d} \sim O(1)$. In studying long wave length collective excitations, the above simplification is well justified. In addition, from dimensional analysis and matching (1.16) to (1.10), we only need to retain derivative terms up quadratic order. So we finally arrive at the following effective Lagrangian:

$$\mathcal{L}_{\text{eff}} = \frac{1}{2K(\mathbf{r})}\left[\frac{1}{\hbar v(\mathbf{r})}(\partial_\tau \theta)^2 + \hbar v(\mathbf{r})(\nabla\theta)^2\right] \tag{1.18}$$

where

$$v(\mathbf{r}) = \sqrt{\frac{g_D \rho_{TF}(\mathbf{r})}{m}} \tag{1.19}$$

can be interpreted as the local velocity of sound. The interaction parameter $K(\mathbf{r})$:

$$K(\mathbf{r}) = \frac{1}{\hbar}\sqrt{\frac{g_D m}{\rho_{TF}(\mathbf{r})}} \tag{1.20}$$

is inhomogeneous due to the confining external potential. It is straightforward to show that the Riemann tensor is non-vanishing, so the effective Lagrangian (1.18) describes a massless scalar phase field $\theta(\mathbf{r},\tau)$ in a curved spacetime. We see the Nambu-Goldstone boson field indeed results from the nonvanishing of order parameter in ground state, which spontaneously breaks the global $U(1)$ symmetry. In 1D and with vanishing external confining potential, the effective Lagrangian(1.18) also describes the Luttinger liquid of interacting fermions. An operator approach to the 1D quantum liquid was given by Haldane [1].

1.2.2 Matsubara Green's Function

To discuss finite temperature correlation and linear response, it is desirable to calculate the Matsubara Green's function defined by

$$\mathcal{G}(\mathbf{r},\tau;\mathbf{r}',\tau') \equiv -\langle \mathcal{T}_\tau \hat{\psi}(\mathbf{r},\tau)\hat{\psi}^\dagger(\mathbf{r}',\tau')\rangle \tag{1.21}$$

where $\mathcal{T}_\tau$ denotes imaginary-time ordering. In the functional representation the Matsubara Green's function can written as:

$$
\begin{aligned}
& \mathcal{G}(\mathbf{r},\tau;\mathbf{r}',\tau') \\
= & -\frac{\int \mathcal{D}\psi^* \mathcal{D}\psi \psi(\mathbf{r},\tau)\psi^*(\mathbf{r}',\tau') e^{-\int_0^\beta d\tau \int d^D r \mathcal{L}[\psi,\psi^*]}}{\int \mathcal{D}\psi^* \mathcal{D}\psi e^{-\int_0^\beta d\tau \int d^D r \mathcal{L}[\psi,\psi^*]}} \\
= & \frac{\int \mathcal{D}\rho \mathcal{D}\theta \sqrt{\rho(\mathbf{r},\tau)\rho(\mathbf{r}',\tau')} e^{i[\theta(\mathbf{r},\tau)-\theta(\mathbf{r}',\tau')]-\int_0^\beta d\tau \int d^D r \mathcal{L}[\rho,\theta]}}{\int \mathcal{D}\rho \mathcal{D}\theta \; e^{-\int_0^\beta d\tau \int d^D r \mathcal{L}[\rho,\theta]}} \\
\approx & -\sqrt{\rho_{TF}(\mathbf{r})\rho_{TF}(\mathbf{r}')} \frac{\int \mathcal{D}\theta e^{i[\theta(\mathbf{r},\tau)-\theta(\mathbf{r}',\tau')]-\int_0^\beta d\tau \int d^D r \mathcal{L}_{\text{eff}}[\theta]}}{\int \mathcal{D}\theta e^{-\int_0^\beta d\tau \int d^D r \mathcal{L}_{\text{eff}}[\theta]}} \\
= & -\sqrt{\rho_{TF}(\mathbf{r})\rho_{TF}(\mathbf{r}')} \langle T_\tau e^{i[\theta(\mathbf{r},\tau)-\theta(\mathbf{r}',\tau')]} \rangle
\end{aligned}
$$

In the second line, we use the fact that the density fluctuation is small (1.13) and therefore can be neglected. Since the effective Lagrangian (1.18) is quadratic in $\theta(\mathbf{r},\tau)$, $\hat{\theta}(\mathbf{r},\tau)$ is a linear function of bosonic operators. For any function of linear bosonic operators we have the identity:

$$\langle e^{\hat{f}_1} e^{\hat{f}_2} \rangle = e^{\langle \hat{f}_1 \hat{f}_2 + \frac{1}{2}(\hat{f}_1{}^2 + \hat{f}_2{}^2) \rangle} \tag{1.22}$$

So the Matsubara Green's function becomes:

$$\mathcal{G}(\mathbf{r},\tau;\mathbf{r}',\tau') = -\sqrt{\rho_{TF}(\mathbf{r})\rho_{TF}(\mathbf{r}')} e^{-F(\mathbf{r},\tau;\mathbf{r}',\tau')} \tag{1.23}$$

and

$$
\begin{aligned}
& F(\mathbf{r},\tau;\mathbf{r}',\tau') \\
= & \mathcal{G}^{(\theta)}(\mathbf{r},\tau;\mathbf{r}',\tau') - \frac{1}{2}\left[\mathcal{G}^{(\theta)}(\mathbf{r},\tau;\mathbf{r},\tau) + \mathcal{G}^{(\theta)}(\mathbf{r}',\tau';\mathbf{r}',\tau')\right]
\end{aligned} \tag{1.24}
$$

We thus reduce the $\hat{\psi}$ field Matsubara Green's function to the calculation of the $\hat{\theta}$ field Matsubara Green's function $\mathcal{G}^{(\theta)}(\mathbf{r},\tau;\mathbf{r}',\tau')$:

$$\mathcal{G}^{(\theta)}(\mathbf{r},\tau;\mathbf{r}',\tau') \equiv -\langle T_\tau \hat{\theta}(\mathbf{r},\tau)\hat{\theta}(\mathbf{r}',\tau') \rangle \tag{1.25}$$

which satisfies:

$$\left[\frac{1}{g_D}\partial_\tau^2 + \frac{\hbar^2}{m}\nabla \cdot (\rho_{TF}(\mathbf{r})\nabla)\right] \mathcal{G}^{(\theta)}(\mathbf{r},\tau;\mathbf{r}',\tau') = \delta(\mathbf{r}-\mathbf{r}')\delta(\tau-\tau') \tag{1.26}$$

For vanishing external confining potential, by appropriate scaling, (1.26) is just the Green's function for D+1 dimensional Poisson equation with periodic boundary condition in the $\hat{\tau}$ direction. For the inhomogeneous case, $\rho_{TF}(\mathbf{r}) \neq$ constant, one should be careful when specifying the boundary condition for $\mathcal{G}^{(\theta)}(\mathbf{r},\tau;\mathbf{r}',\tau')$ [6]. Since we are working at length scales no shorter than the healing length (1.17), there is ambiguity in the regions where $\rho_{TF}(\mathbf{r}) = 0$. It is natural to impose the natural boundary condition:

$$|\mathcal{G}^{(\theta)}(\mathbf{r},\tau;\mathbf{r}',\tau')| < \infty \tag{1.27}$$

from the fact that ψ and its normal derivatives are bounded.

1.3 Matusbara Green's Function for Bose Gases in Harmonic Traps

1.3.1 1D Trapped Bose Gases

The correlation function for an unconfined 1D quantum fluid has been discussed extensively in the literature [1, 1, 24]. The problem of homogeneous interacting bosons can be related to the problem of interacting fermions by Jordan-Wigner transformation [22] and they both can be described by the same effective Lagrangian (1.18), except for possible redefinition of parameters. We simply have to solve:

$$\frac{1}{K}\left(\frac{1}{\hbar v}\partial_\tau^2 + \hbar v \partial_r^2\right) \mathcal{G}^{(\theta)}(r,\tau;r',\tau') = \delta(r-r')\delta(\tau-\tau') \tag{1.28}$$

which, with (1.24) inserted into (1.23), yields

$$\mathcal{G}(r,\tau;r',\tau') = -\frac{\rho}{\left|\frac{\beta\hbar v}{\pi d}\sinh\left[\frac{\pi}{\beta\hbar v}[|r-r'| + i\hbar v(\tau-\tau') + d]\right]\right|^{\frac{1}{\gamma}}} \tag{1.29}$$

with gas density $\rho = \frac{\mu}{g_1}$, velocity of sound

$$v = \sqrt{\frac{g_1 \rho}{m}} \tag{1.30}$$

and interaction parameter

$$K = \frac{1}{\hbar}\sqrt{\frac{g_1 m}{\rho}} \tag{1.31}$$

d is a short distance cutoff parameter, which regularizes the theory. The scaling exponent:

$$\gamma = \frac{2\pi}{K} = \frac{2\pi\hbar\rho}{mv} \tag{1.32}$$

has pure quantum nature even at finite temperatures. The one-body density matrix

$$n(\mathbf{r},\mathbf{r}') = -\mathcal{G}(\mathbf{r},\tau;\mathbf{r}',\tau+0^+) \tag{1.33}$$

which characterizes long-range order, decays exponentially at finite temperature:

$$n(r,r') \propto e^{-\frac{|r-r'|}{\lambda(T)}} \tag{1.34}$$

where the coherence length is found to be

$$\lambda(T) = \frac{2\hbar^2\rho}{mk_BT} \tag{1.35}$$

Obviously, there is no quantum degeneracy when $\lambda(T) < \frac{1}{\rho}$, which sets an upper bound for (1.29) to hold:

$$T < \frac{\hbar^2\rho^2}{2mk_B} \tag{1.36}$$

At $T \to 0$, however, there exists quasi long-range order since $n(r, r')$ decays as a power law. The zero temperature Green's function is given by:

$$G(r, t; r', t') = \langle \mathcal{T} \hat{\psi}(r, t) \hat{\psi}^\dagger(r', t') \rangle = \frac{\rho}{\left| \frac{1}{d} \left[|r - r'| - v(t - t') + d \right] \right|^{\frac{1}{\gamma}}} \tag{1.37}$$

which shows the feature of Lorentz invariance of the effective Lagrangian. The speed of light is replaced by the velocity of sound and the correlation function decays as a power law.

Now let us consider a harmonic external confining potential:

$$V_{\text{ext}}(r) = \frac{1}{2} m \omega_z^2 r^2 \tag{1.38}$$

Since the effective Lagrangian approach is only valid under the condition (1.13), it is necessary to find the classical turning point(surface) $\vec{R}_c$ set by

$$V_{\text{ext}}(\vec{R}_c) = \mu \tag{1.39}$$

Physically $\vec{R}_c$ determines the size of the condensate within TFA. For 1D and the harmonic potential (1.38):

$$R_c = \sqrt{\frac{2\mu}{m\omega_z^2}} \tag{1.40}$$

Define dimensionless parameters:

$$x = \frac{r}{R_c} \tag{1.41a}$$

$$\alpha = \frac{2\sqrt{2}\pi}{\beta \hbar \omega_z} \tag{1.41b}$$

then

$$\rho_{TF}(r) = \frac{\mu}{g_1}(1 - x^2)\vartheta(1 - |x|) \tag{1.42}$$

Perform a mode expansion:

$$\mathcal{G}^{(\theta)}(r, \tau; r', \tau') = \frac{1}{\beta} \sum_{\omega_n} e^{-i\omega_n(\tau - \tau')} \tilde{\mathcal{G}}^{(\theta)}(r, r', \omega_n) \tag{1.43}$$

where $\omega_n = \frac{2\pi n}{\beta}$ is the Matsubara frequency for bosons, and substitute (1.42) (1.43) to (1.26), we get:

$$\left[(1-x^2)\partial_x^2 - 2x\partial_x - n^2\alpha^2\right] g(x,x',n\alpha) = \delta(x-x'), \quad |x| \leq 1 \tag{1.44}$$

where

$$g(x,x',n\alpha) = \frac{h^2\omega_z^2 R_c}{2g_1}\tilde{\mathcal{G}}^{(\theta)}(r,r',\omega_n) \tag{1.45}$$

The homogeneous equation to (1.44) is the Legendre equation. The boundary condition (1.27) requires the following eigenfunction expansion:

$$g(x,x',n\alpha) = \sum_{m=0}^{\infty} C_m(x',n\alpha)P_n(x) \tag{1.46}$$

where $P_n(x)$ is the n^{th} Legendre polynomial. Notice that

$$\delta(x-x') = \sum_{m=0}^{\infty}\left(m+\frac{1}{2}\right)P_m(x)P_m(x')$$

We obtain:

$$g(x,x',n\alpha \neq 0) = -\sum_{m=0}^{\infty}\frac{m+\frac{1}{2}}{m(m+1)+n^2\alpha^2}P_m(x)P_m(x') \tag{1.47a}$$

$$g(x,x',n\alpha = 0) = \frac{1}{2} - \sum_{m=1}^{\infty}\frac{m+\frac{1}{2}}{m(m+1)}P_m(x)P_m(x') \tag{1.47b}$$

The $n=0$ mode (1.47b) corresponds to static correlation. Substituting (1.47b) into (1.43) and performing the sum exactly[25], we obtain the static phase field Matsubara Green's function:

$$\begin{aligned} & \mathcal{G}_s^{(\theta)}(r,r') \\ \equiv\ & \frac{1}{\beta}\tilde{\mathcal{G}}^{(\theta)}(r,r',\omega_n=0) \\ =\ & \frac{1}{\delta(T)}\ln\left[\left(1+\frac{|r-r'|}{2R_c}\right)^2 - \left(\frac{|r+r'|}{2R_c}\right)^2\right] \end{aligned} \tag{1.48}$$

which contributes to the static part of (1.24):

$$F_s(r,r') = \frac{1}{2\delta(T)}\left|\ln\left[\frac{\left(1-\frac{r}{R_c}\right)\left(1+\frac{r'}{R_c}\right)}{\left(1+\frac{r}{R_c}\right)\left(1-\frac{r'}{R_c}\right)}\right]\right| \tag{1.49}$$

where

$$\delta(T) = \frac{2\hbar^2\rho_{TF}(0)}{mk_BTR_c} = \frac{\lambda(T)}{R_c} \tag{1.50}$$

$\lambda(T)$ is the coherence length defined in (1.35). Due to finite size of the sample, it is possible to define a characteristic temperature T_θ [26] such that $\lambda(T_\theta) = R_c$, i.e.

$$T_\theta = \frac{2\hbar^2\rho_{TF}(0)}{mk_BR_c} \tag{1.51}$$

At $T < T_\theta$, the coherence length exceeds the sample size R_c, and both density and phase fluctuations are suppressed. A true condensate can be realized. Notice that $F_s(r,r')$ in (1.49) agrees exactly with that obtained by the hydrodynamic approach [8]. A similar expression was given by Bogoliubov *et al.* [16] using the functional method; however, their results have a different expression for the velocity of sound.

The dynamic part (1.47a) can also be summed exactly to give:

$$\tilde{\mathcal{G}}_d^{(\theta)}(r,r',\omega_n) = \frac{g_1\pi}{\hbar^2\omega_z^2R_c\sin(\nu_n\pi)}P_{\nu_n}\left(\frac{r_>}{R_c}\right)P_{\nu_n}\left(-\frac{r_<}{R_c}\right) \tag{1.52}$$

where

$$\nu_n = -\frac{1}{2} + \sqrt{\frac{1}{4} - n^2\alpha^2} \tag{1.53}$$

and $r_> \equiv \max\{r,r'\}$, $r_< \equiv \min\{r,r'\}$. $P_{\nu_n}(x)$ is the Legendre function of the first kind. It is well known that by analytic continuation, $i\omega_n \to E + i\delta$, the Matsubara Green's function becomes the retarded Green's function, whose poles give energy spectrum. From (1.52), we see that these poles are located at $\nu_n = m,\ m = 0,1,2,\cdots$. So the energy spectrum is

$$E_m = \hbar\omega_z\sqrt{\frac{m(m+1)}{2}}, \quad m = 0,1,2,\cdots \tag{1.54}$$

This result agrees with [16] but different from that of [4, 6] for quasi-1D trapped gas:

$$E_m = \frac{1}{2}\hbar\omega_z\sqrt{m(m+3)} \tag{1.55}$$

The difference is due to the average over radial degrees of freedom of the latter work.

For temperatures:

$$T > \frac{\hbar\omega_z}{2\sqrt{2}\pi k_B} \tag{1.56}$$

we have $|\nu_n| > 1$ and we are justified to use the following expansion [19]:

$$P_\nu(\cos\varphi) = \sqrt{\frac{2}{\nu\pi\sin\varphi}}\cos\left[\left(\nu+\frac{1}{2}\right)\varphi - \frac{\pi}{4}\right] + O\left(\frac{1}{\sqrt{\nu^3}}\right) \tag{1.57}$$

with $0 < \epsilon \le \varphi \le \pi - \epsilon$; $\nu \gg \frac{1}{\epsilon}$, or equivalently, $r, r' \ll R_c$. In fact, this expansion can be applied to much lower temperatures and $r, r' \sim R_c$ for the following reasons:(1)Large $|\nu_n|$ can also be ensured by large n in (1.53), so the expansion (1.57) works better for higher modes;(2)The TFA breaks down near the trap edge, so errors in extending r, r' to R_c would be within that of TFA. To order $\left(\frac{r}{R_c}\right)^2$, we find

$$\tilde{\mathcal{G}}_d^{(\theta)}(r, r', \omega_n) = -\frac{2g_1 e^{-|n|\alpha\pi}}{\hbar^2\omega_z^2\alpha\sigma(r,r')R_c|n|}\cosh\left[|n|\alpha\left(\pi - \frac{|r-r'|}{R_c}\right)\right] \tag{1.58}$$

where

$$\sigma(r, r') = \frac{1}{2} + \frac{\rho_{TF}(r) + \rho_{TF}(r')}{4\rho_{TF}(0)} \tag{1.59}$$

Substitution of (1.58) to (1.43) leads to a dynamic correlation function:

$$\begin{aligned} \mathcal{G}_d^{(\theta)}(r, \tau; r', \tau') &= \frac{1}{\gamma(r,r')}\ln\left|\frac{\beta\hbar v(0)}{\pi d}\sinh\left[\frac{\pi}{\beta\hbar v(0)}[|r-r'| + i\hbar v(0)(\tau-\tau') + d]\right]\right| \\ &+ \frac{1}{\gamma(r,r')}\ln\left|\frac{\beta\hbar v(0)}{\pi d}\sinh\left[\frac{\pi}{\beta\hbar v(0)}[2\pi R_c - |r-r'| + i\hbar v(0)(\tau-\tau')]\right]\right| \end{aligned} \tag{1.60}$$

with a spatially-dependent coefficient

$$\gamma(r, r') = \frac{2\pi\hbar\rho_{TF}(0)\sigma(r, r')}{mv(0)} \tag{1.61}$$

It is clear that in the limit $R_c \to \infty$, $\gamma(r, r')$ reduces to the result of untrapped gas (1.32). The phase field Green's function

$$\mathcal{G}^{(\theta)}(r, \tau; r', \tau') = \mathcal{G}_s^{(\theta)}(r, r') + \mathcal{G}_d^{(\theta)}(r, \tau; r', \tau') \tag{1.62}$$

together with (1.23) and (1.24), yields the following Matsubara Green's function for 1D trapped bosons in a harmonic potential:

$$\begin{aligned} \mathcal{G}(r, \tau; r', \tau') &= -\frac{\sqrt{\zeta(r, r', T)}}{\left|\frac{\beta\hbar v(0)}{\pi d}\sinh\left[\frac{\pi}{\beta\hbar v(0)}[|r - r'| + i\hbar v(0)(\tau - \tau') + d]\right]\right|^{\frac{1}{\gamma(r,r')}}} \\ &\times \frac{1}{\left|\frac{\beta\hbar v(0)}{\pi d}\sinh\left[\frac{\pi}{\beta\hbar v(0)}[2\pi R_c - |r - r'| + i\hbar v(0)(\tau - \tau')]\right]\right|^{\frac{1}{\gamma(r,r')}}} \end{aligned} \tag{1.63}$$

where

$$\zeta(r, r', T) = \rho_{TF}(r)\rho_{TF}(r') \exp\left\{-\frac{1}{\delta(T)}\left|\ln\left[\frac{\left(1 - \frac{r}{R_c}\right)\left(1 + \frac{r'}{R_c}\right)}{\left(1 + \frac{r}{R_c}\right)\left(1 - \frac{r'}{R_c}\right)}\right]\right|\right\} \tag{1.64}$$

is the renormalized static density correlation function, which comes directly from the static contribution of the phase field $F_s(r, r')$. Note the following features of trapped 1D boson gases: (a) At finite temperatures, the off-diagonal long range order $n(r, r')$ is determined by static density correlations, while for untrapped gases it is the dynamic correlation that contributes. Indeed, expanding $\zeta(r, r', T)$ to lowest order in $\frac{r}{R_c}$ and $\frac{r'}{R_c}$ gives

$$n(r, r') \sim e^{-\frac{|r-r'|}{\lambda(T)}} \tag{1.65}$$

which has the same form as untrapped gases (1.34). Close to the edge of the trap, $n(r, r')$

decays faster than this exponential behavior as seen from the logarithm in (1.64). Physically this can be understood because in the vicinity of trap edge, the healing length is much larger than in the trap center, so the actual condensate size is smaller than R_c; (b) At $T = 0$, only the dynamic $F_d(r, \tau; r', \tau')$ contributes to $\mathcal{G}(r, \tau; r', \tau')$. The inhomogeneity shows up as a spatial-dependent exponent (1.61), which involves an average over the condensate density at r and r'. This spatial-dependence, which is absent in untrapped gases, is a higher order effect and it is difficult to detect if the analysis is restricted to the region of trap center. In fact, as $R_c \to \infty$, $F_s(r, r')$ vanishes, and the second term in $\mathcal{G}_d^{(\theta)}(r, \tau; r', \tau')$ (1.60) becomes a constant and does not contribute to $F_d(r, \tau; r', \tau')$. So $\mathcal{G}(r, \tau; r', \tau')$ (1.63) would only include the first term thereby reducing to the Matsubara Green's function of untrapped 1D Bose gases (1.29), as it should.

It is useful to compare our results for 1D trapped Bose gases with that obtained by the hydrodynamic approach, for example,[8, 26] and the functional approach of successive integration of fast modes (SIFM) recently adopted by Bogoliubov *et al.*[16]. We find that (a) our results agree exactly with hydrodynamic approach for the static correlation function and condensate parameters such as condensate density and velocity of sound, but are different from that obtained from SIFM; (b) in the quasi-homogeneous limit, our results for the dynamic correlation reduce to the same functional form as that obtained by SIFM. However, our spatial-dependent exponent $\gamma(r, r')$ (1.61) depends on an inhomogeneity expansion parameter

$$\frac{\rho_{TF}(r) + \rho_{TF}(r')}{4\rho_{TF}(0)} \tag{1.66}$$

whereas in SIFM the exponent depends on condensate density at $\rho_{TF}(\frac{r+r'}{2})$ only. Unfortunately, analytic results from hydrodynamic approach are not available for comparison so far; (c) we find that static and dynamic correlation play different roles in the off-diagonal long range order for trapped 1D Bose gases at different temperatures, while SIFM suggests that only dynamic correlation contributes. In principle, within the TFA, all approaches should give the same results for physical quantities. We think the discrepancies arise mainly from technical aspects: In SIFM, one must first integrate over fast modes *exactly* to obtain an effective Lagrangian. This is practically not possible due to the new vertices generated by interaction [13]. So any particular approximation made in this early stage would inevitably introduce uncertainty in the renormalized coupling parameters like condensate density, velocity of sound and so on, which bring about the differences in the final results. A second factor that accounts for the discrepancies comes from boundary conditions. We find it physically appealing to use the natural boundary condition (1.27).

1.3.2 2D Trapped Bose Gases

Now let us consider a 2D Bose gas confined in a harmonic potential:

$$V_{\text{ext}}(\mathbf{r}) = \frac{1}{2} m\omega_{\perp}^2 r^2 \tag{1.67}$$

where $\omega_{\perp}$ is the radial trapping frequency. The classical turning surface is found to be:

$$R_c = \sqrt{\frac{2\mu}{m\omega_{\perp}^2}} \tag{1.68}$$

The condensate density is:

$$\rho_{TF}(\mathbf{r}) = \frac{\mu}{g_2}(1 - x^2)\vartheta(1 - x) \tag{1.69}$$

where $x = \frac{r}{R_c}$. In cylindrical polar coordinates

$$\nabla = \partial_r \hat{e}_r + \frac{1}{r}\partial_\phi \hat{e}_\phi \tag{1.70a}$$

$$\nabla^2 = \frac{1}{r}\partial_r(r\partial_r) + \frac{1}{r^2}\partial_\phi^2 \tag{1.70b}$$

$$\delta(\mathbf{r} - \mathbf{r}') = \frac{1}{r}\delta(r - r')\delta(\phi - \phi') \tag{1.70c}$$

(1.26) becomes:

$$\begin{aligned}
&\left\{\frac{1}{g_2}\partial_\tau^2 + \frac{\hbar^2\rho_{TF}(\mathbf{r})}{m}\left[\frac{1}{r}\partial_r(r\partial_r) + \frac{1}{r^2}\partial_\phi^2\right] + \frac{\hbar^2}{m}\partial_r\rho_{TF}(\mathbf{r})\partial_r\right\}\mathcal{G}^{(\theta)}(\mathbf{r},\tau;\mathbf{r}',\tau') \\
= \;& \frac{1}{r}\delta(\tau-\tau')\delta(r-r')\delta(\phi-\phi') \qquad (1.71)
\end{aligned}$$

Substitution of mode expansion:

$$\mathcal{G}^{(\theta)}(\mathbf{r},\tau;\mathbf{r}',\tau') = \frac{1}{2\pi\beta}\sum_{\omega_n}\sum_{l} e^{-i\omega_n(\tau-\tau')+il(\phi-\phi')}\tilde{\mathcal{G}}^{(\theta)}(r,r',\omega_n,l) \qquad (1.72)$$

to (1.71) leads to:

$$\left\{(1-x^2)\left[\frac{1}{x}\partial_x(x\partial_x) - \frac{l^2}{x^2}\right] - 2x\partial_x - n^2\alpha^2\right\}g(x,x',n\alpha,l) = \frac{1}{x}\delta(x-x') \qquad (1.73)$$

where

$$\alpha = \frac{2\sqrt{2}\pi}{\beta\hbar\omega_\perp} \qquad (1.74a)$$

$$g(x,x',n\alpha,l) = \frac{\hbar^2\mu}{g_2 m}\tilde{\mathcal{G}}^{(\theta)}(r,r',\omega_n,l) \qquad (1.74b)$$

To find the Green's function, we first solve the following equation:

$$\left\{(1-x^2)\left[\frac{1}{x}\frac{d}{dx}\left(x\frac{d}{dx}\right) - \frac{l^2}{x^2}\right] - 2x\frac{d}{dx} - \lambda^2\right\}u_l(x) = 0 \qquad (1.75)$$

The eigenfunctions of the equation (1.93) can be found in a series form:

$$u_l(x) = \sum_{m=0}^{\infty} c_{2m}x^{2m+|l|} \qquad (1.76)$$

with the following recursion relation for the coefficients:

$$c_{2m+2} = \frac{(2m+l)^2 + 2(2m+l) - l^2 - \lambda^2}{(2m+2)(2m+2l+2)}c_{2m} \qquad (1.77)$$

It is clear that the series would reduce to a polynomial of order n if

$$\lambda^2 = n^2 + 2n - l^2 \tag{1.78}$$

with $n = 2m + l$. We obtain the following eigenfunction:

$$u_{n,l}(x) = \sum_{m=0}^{\frac{n-|l|}{2}} c_{2m} x^{2m+|l|} \tag{1.79}$$

with c_0 is an undetermined coefficient. By analytic continuation $i\omega_n = E + i\delta$, we obtain the energy spectrum for 2D trapped Bose gases [18] from (1.73) and (1.78):

$$E_{n,l} = \hbar\omega_\perp \sqrt{\frac{n^2 + 2n - l^2}{2}}, \quad n \geq |l| \tag{1.80}$$

The Green's function $g(x, x', n\alpha, l)$ can be constructed from the eigenfunctions $\{u_{n,l}(x)\}$. However, unlike 1D, where phase space is so restricted, it is usually difficult to obtain an analytic expression in higher dimension. On the other hand, if we are interested in regions: $|\mathbf{r}| \ll R_c$, certain approximation can be made to (1.26). Notice that: (a) if there is no confining potential, then $\rho_{TF}(\mathbf{r}) = \rho_{TF}(0)$ is a constant and (1.26) is Poisson equation with periodic boundary condition, which is exactly solvable; (b) $\nabla\rho_{TF}(\mathbf{r})$ is only significant at $|\mathbf{r}| \sim R_c$, so it can be neglected for regions $|\mathbf{r}| \ll R_c$; (c) $\mathcal{G}^{(\theta)}(\mathbf{r}, \tau; \mathbf{r}', \tau')$ is symmetric with respect to its argument. So we are led to the following approximat equation:

$$\left[\frac{1}{g_D}\partial_\tau^2 + \frac{\hbar^2\rho_{TF}(0)\sigma(\mathbf{r}, \mathbf{r}')}{m}\nabla^2\right] \mathcal{G}^{(\theta)}(\mathbf{r}, \tau; \mathbf{r}', \tau') = \delta(\mathbf{r} - \mathbf{r}')\delta(\tau - \tau') \tag{1.81}$$

where $\sigma(\mathbf{r}, \mathbf{r}')$ is a small parameter with the following properties: (a) $\sigma(\mathbf{r}, \mathbf{r}')$ is symmetric with respect to $\mathbf{r}$ and $\mathbf{r}'$; (b) $0 < \sigma(\mathbf{r}, \mathbf{r}') \leq 1$. The equality holds when there is no confining potential; (3) $\sigma(\mathbf{r}, \mathbf{r}')$ is small and smooth, so it is not subject to differentiation in this order of calculation. To find $\sigma(\mathbf{r},\mathbf{r}')$, define $\mathbf{r}_c = \frac{\mathbf{r}+\mathbf{r}'}{2}$ and $\mathbf{R} = \mathbf{r} - \mathbf{r}'$. In the limit $|\mathbf{r}|, |\mathbf{r}'| \ll R_c$:

$$\begin{aligned}
\rho_{TF}(\mathbf{r}) &= \rho_{TF}\left(\mathbf{r}_c + \frac{\mathbf{R}}{2}\right) \\
&= \frac{1}{2}\left[\rho_{TF}(\mathbf{r}_c) + \rho_{TF}\left(\frac{\mathbf{R}}{2}\right)\right] + O\left(\max\left(\frac{\mathbf{r}_c}{R_c}, \frac{\mathbf{R}}{2R_c}\right)^2\right) \\
&\approx \rho_{TF}(0)\left[\frac{1}{2} + \frac{\rho_{TF}(\mathbf{r}) + \rho_{TF}(\mathbf{r}')}{4\rho_{TF}(0)}\right] \\
&= \rho_{TF}(0)\sigma(\mathbf{r},\mathbf{r}') \qquad (1.82)
\end{aligned}$$

We see $\sigma(\mathbf{r},\mathbf{r}')$ takes exactly the same form as that obtained from 1D analytic calculation(1.59).

Now we use the simplified equation (1.81) to calculate $\mathcal{G}^{(\theta)}(\mathbf{r},\tau;\mathbf{r}',\tau')$ for trapped Bose gases in 2D. Using the mode expansion (1.72), (1.81) becomes:

$$\left[\partial_x^2 + \frac{1}{x}\partial_x - \left(n^2\tilde{\alpha}^2 + \frac{l^2}{x^2}\right)\right] g_<(x,x',n\tilde{\alpha},l) = \frac{1}{x}\delta(x-x') \qquad (1.83)$$

where

$$\tilde{\alpha} = \frac{2\pi R_c}{\beta\hbar\tilde{v}} \qquad (1.84a)$$

$$\tilde{v} = v(0)\sqrt{\sigma(\mathbf{r},\mathbf{r}')} \qquad (1.84b)$$

$$g_<(x,x',n\tilde{\alpha},l) = \frac{\hbar^2\rho_{TF}(0)\sigma(\mathbf{r},\mathbf{r}')}{m}\tilde{\mathcal{G}}^{(\theta)}(r,r',\omega_n,l) \qquad (1.84c)$$

By imposing natural boundary condition (1.27), we find:

$$g_{<,d}(x,x',n\tilde{\alpha},l) = -I_l(|n|\tilde{\alpha}x_<)K_l(|n|\tilde{\alpha}x_>)\ , \quad n\tilde{\alpha} \neq 0 \qquad (1.85a)$$

$$g_{<,s}(x,x',l=0) = \ln x_>\ , \quad n\tilde{\alpha} = 0 \qquad (1.85b)$$

$$g_{<,s}(x,x',l\neq 0) = -\frac{1}{2|l|}\left(\frac{x_<}{x_>}\right)^{|l|}\ , \quad n\tilde{\alpha} = 0 \qquad (1.85c)$$

where $I_l(z)$ and $K_l(z)$ are modified Bessel functions of first and second kind respectively.

Substituting (1.84) and (1.85) into (1.72) and performing the sum exactly, we find:

$$\mathcal{G}_s^{(\theta)}(\mathbf{r},\mathbf{r}') = \frac{g_2}{2\pi\beta\hbar^2\tilde{v}^2}\ln\left(\frac{|\mathbf{r}-\mathbf{r}'|}{R_c}\right) \tag{1.86}$$

$$\begin{aligned} & \mathcal{G}_d^{(\theta)}(\mathbf{r},\tau;\mathbf{r}',\tau') \\ = & -\frac{g_2}{4\pi\hbar\tilde{v}}\sum_{k=1}^{\infty}\left[\frac{1}{\sqrt{(\mathbf{r}-\mathbf{r}')^2+\hbar^2\tilde{v}^2[k\beta-(\tau-\tau')]^2}}-\frac{1}{k\beta\hbar\tilde{v}}\right] \\ - & \frac{g_2}{4\pi\hbar\tilde{v}}\sum_{k=1}^{\infty}\left[\frac{1}{\sqrt{(\mathbf{r}-\mathbf{r}')^2+\hbar^2\tilde{v}^2[k\beta+(\tau-\tau')]^2}}-\frac{1}{k\beta\hbar\tilde{v}}\right] \\ - & \frac{g_2}{4\pi\hbar\tilde{v}}\frac{1}{\left||\mathbf{r}-\mathbf{r}'|+i\hbar\tilde{v}(\tau-\tau')\right|}-\frac{g_2}{2\pi\beta\hbar^2\tilde{v}^2}\ln\left(\frac{|\mathbf{r}-\mathbf{r}'|}{2\beta\hbar\tilde{v}}\right) \end{aligned} \tag{1.87}$$

Define $z \equiv |\mathbf{r}-\mathbf{r}'| + i\hbar\tilde{v}(\tau-\tau')$ and examine the asymptotic behavior of $\mathcal{G}^{(\theta)}(\mathbf{r},\tau;\mathbf{r}',\tau') = \mathcal{G}_s^{(\theta)}(\mathbf{r},\mathbf{r}') + \mathcal{G}_d^{(\theta)}(\mathbf{r},\tau;\mathbf{r}',\tau')$:

(a) $|z| < \beta\hbar\tilde{v}$

This limit corresponds to the case when temperature is sufficient low or $(\mathbf{r},\tau)$, $(\mathbf{r}',\tau')$ are close to each other, so only the third term of (1.87) contributes:

$$\mathcal{G}^{(\theta)}(\mathbf{r},\tau;\mathbf{r}',\tau') = -\frac{g_2}{4\pi\hbar\tilde{v}}\frac{1}{\left||\mathbf{r}-\mathbf{r}'|+i\hbar\tilde{v}(\tau-\tau')\right|} \tag{1.88}$$

and the Matsubara Green's function for 2D trapped Bose gases is:

$$\mathcal{G}(\mathbf{r},\tau;\mathbf{r}',\tau') = -\sqrt{\rho_{TF}(\mathbf{r})\rho_{TF}(\mathbf{r}')}\exp\left\{-\frac{g_2}{4\pi\hbar\tilde{v}}\left(\frac{1}{d}-\frac{1}{\left||\mathbf{r}-\mathbf{r}'|+d+i\hbar\tilde{v}(\tau-\tau')\right|}\right)\right\} \tag{1.89}$$

It is clear that as $|\mathbf{r}-\mathbf{r}'| \to \beta\hbar\tilde{v}$, the long-range order is not destroyed and there is true BEC. The short distance divergence is regulated by a short distance cutoff parameter d, which can be taken as the healing length $\xi(\mathbf{r})$ or the average inter-particle distance. There are two main features for the off-diagonal long-range order in this limit: First, the correlation is almost a constant for the condensate, and the correlation length depends on temperature only through the upper bound for this limit to hold, i.e. $|\mathbf{r}-\mathbf{r}'| < \beta\hbar\tilde{v}$. Above this scale the correlation follows a power law decay as will be shown shortly. Qualitatively, the coherence length in this limit goes inversely with temperature. Second, (1.89) shows that particle interaction reduces the coherence length of the condensate in this temperature regime. In fact, the condensate density (1.11) is inversely proportional to interaction strength g_2, so strong particle interaction would decrease the condensate density and therefore reduce the coherence length. This effect has been recently confirmed by numerical results of Hutchinson *et al.* [11]. They found that in the scaled unit of the condensate size, the particle interactions *always* reduce the range of coherence.

(b)$\beta\hbar\tilde{v} \ll |z|$ and $|\mathbf{r}-\mathbf{r}'| \ll 2R_c$

This limit corresponds to correlation at finite temperatures or distant $(\mathbf{r},\tau)$ and $(\mathbf{r}',\tau')$. In this case the leading contributions are the first and second terms in (1.87) and the two sums can be replaced by integrals. We have

$$\mathcal{G}^{(\theta)}(\mathbf{r},\tau;\mathbf{r}',\tau') = \frac{m}{2\pi\beta\hbar^2\rho_{TF}(0)\sigma(\mathbf{r},\mathbf{r}')} \ln\frac{||\mathbf{r}-\mathbf{r}'| + i\hbar\tilde{v}(\tau-\tau')|}{\beta\hbar\tilde{v}} \tag{1.90}$$

and

$$\mathcal{G}(\mathbf{r},\tau;\mathbf{r}',\tau') = -\sqrt{\rho_{TF}(\mathbf{r})\rho_{TF}(\mathbf{r}')}\left(\frac{\beta\hbar\tilde{v}}{||\mathbf{r}-\mathbf{r}'| + i\hbar\tilde{v}(\tau-\tau')|}\right)^{\frac{1}{\gamma_2(\mathbf{r},\mathbf{r}')}} \tag{1.91}$$

where the exponent of the power law is:

$$\gamma_2(\mathbf{r},\mathbf{r}') = \frac{2\pi\beta\hbar^2\rho_{TF}(0)\sigma(\mathbf{r},\mathbf{r}')}{m} \tag{1.92}$$

It is clear that the exponent explicitly depends on thermal fluctuations. This is different from 1D case (c.p.(1.61)), where the fluctuation is entirely of quantum nature. In both cases, the exponents are spatially-dependent due to the confining potential, as can be seen from the appearance of the inhomogeneity parameter $\sigma(\mathbf{r},\mathbf{r}')$. In this limit, the off-diagonal long-ranger order decays as a power law and its temperature-dependence is complicated. The particle interaction affects the coherence length through the condensate density in the exponent $\gamma_2(\mathbf{r},\mathbf{r}')$, and therefore strong interactions will reduce the coherence of Bose gases in this finite-temperature region, i.e. we have shown that particle interaction(repulsive) always reduces the coherence.

1.4 Conclusions

In this chapter, we have derived an effective Lagrangian for trapped Bose gases at low temperatures. The key idea is to apply the Goldstone theorem to identify the Nambu-Goldstone field as an effective field for low energy excitations. The structure of the effective field theory is determined by $U(1)$ symmetry transformation of the original field, while the coefficients are determined by a matching procedure. In this way, we are able to incorporate various commonly adopted approximations in a coherent way. The functional approach shows that the standard quantized hydrodynamic approach, which is based on the GP equation, corresponds to a quantum correction around a semiclassical configuration. Both approaches are valid only for weakly interacting Bose gases.

Using the effective Lagrangian, we have calculated the Matsubara Green's function of trapped 1D and 2D Bose gases. For 1D gases, we are able to compare our results with that obtained by the hydrodynamic approach and the functional approach of SIFM. We find that the natural boundary condition is physically appealing and suitable for the Matsubara Green's function calculation. Our results agree well with that obtained by the hydrodynamic approach, while they differ from SIFM results. This difference comes mainly from the difficulty of integrating fast modes in the early stages of SIFM. We believe that the effective Lagrangian approach is a direct and efficient approach to low energy excitation of trapped Bose gases. Unlike 1D, the analytic calculation for trapped Bose gases in 2D and higher dimensions is generally difficult due to inhomogeneous nature of the condensate. We suggest a possible simplification scheme and apply it to the 2D gases. We find that both the scaling exponent and the velocity of sound are renormalized by the inhomogeneity parameter $\sigma(\mathbf{r}, \mathbf{r}')$, consistent with our 1D results. Finally, we study the role of particle interaction in coherence property of 2D condensate. Theoretical calculations show that particle interaction always decreases the coherence of trapped Bose gases in 2D due to the decreasing of condensate density and increasing of healing length.

1.5 Appendix A: Calculation of Energy Spectrum of 2D Trapped Bose Gases

I include the calculation of the energy spectrum of 2D trapped Bose gases in this appendix. The following differential equation has to be solved:

$$\left\{(1-x^2)\left[\frac{1}{x}\frac{d}{dx}\left(x\frac{d}{dx}\right)-\frac{l^2}{x^2}\right]-2x\frac{d}{dx}+\mu^2\right\}u_l(x)=0 \tag{1.93}$$

In a standard form it becomes:

$$u''(x)+p(x)u'(x)+q(x)u(x)=0 \tag{1.94}$$

with

$$p(x)=\frac{1}{x}-\frac{2x}{1-x^2} \tag{1.95a}$$

$$q(x)=\frac{\mu^2}{1-x^2}-\frac{l^2}{x^2} \tag{1.95b}$$

It is clear $x=0$ is a regular singularity point so I look for series solution around $x=0$:

$$u(x)=\sum_{n=0}^{\infty}c_n x^{n+s} \tag{1.96a}$$

$$p(x)=\sum_{n=0}^{\infty}a_n x^{n-1} \tag{1.96b}$$

$$q(x)=\sum_{n=0}^{\infty}b_n x^{n-2} \tag{1.96c}$$

$$p(x)=\frac{1}{x}-\frac{2x}{1-x^2}=\frac{1}{x}-2x-2x^3-\cdots-2x^{2n+1}-\cdots \tag{1.97}$$

so

$$a_k = \begin{cases} 0 & k = 2n-1, \qquad n = 1, 2, \cdots \\ 1 & k = 0 \\ -2 & k = 2n, \qquad n = 1, 2, \cdots \end{cases} \tag{1.98}$$

$$q(x) = \frac{\mu^2}{1-x^2} - \frac{l^2}{x^2} = -l^2 x^{-2} + \mu^2 + \mu^2 x^2 + \cdots + \mu^2 x^{2n} + \cdots \tag{1.99}$$

thus

$$b_k = \begin{cases} 0 & k = 2n-1, \qquad n = 1, 2, \cdots \\ -l^2 & k = 0 \\ \mu^2 & k = 2n, \qquad n = 1, 2, \cdots \end{cases} \tag{1.100}$$

Substituting (1.96) to (1.94) leads to

$$\sum_{n=0}^{\infty}(n+s)(n+s-1)c_n x^{n+s-2} + \sum_{k=0}^{\infty} a_k x^{k-1} \sum_{n=0}^{\infty}(n+s)c_n x^{n+s-1} + \sum_{k=0}^{\infty} b_k x^{k-2} \sum_{n=0}^{\infty} c_n x^{n+s} = 0 \tag{1.101}$$

The coefficients of the series must vanish:

$\boxed{x^{s-2}}$ -indicial equation

$$s(s-1) + s - l^2 = 0 \tag{1.102}$$

so

$$s = l \tag{1.103}$$

$\boxed{x^{s-1}}$

$$\left[l(l+1) + (l+1) - l^2\right] c_1 = 0 \tag{1.104}$$

so

$$c_1 = 0 \tag{1.105}$$

$\boxed{x^s}$

$$(l+1)(l+2)c_2 + la_2c_0 + (l+2)a_0c_2 + b_2c_0 + b_0c_2 = 0 \tag{1.106}$$

so

$$c_2 = \frac{2l-\mu^2}{4(l+1)}c_0 \tag{1.107}$$

$\boxed{x^{s+1}}$

$$\left[(l+2)(l+3)+(l+3)-l^2\right]c_3 = 0 \tag{1.108}$$

so

$$c_3 = 0 \tag{1.109}$$

$\boxed{x^{2k+s}}$

$$4(k+1)(k+l+1)c_{2k+2} - 2\left[lc_0 + (l+2)c_2 + \cdots + (l+2k)c_{2k}\right] + \mu^2(c_0 + c_2 + \cdots + c_{2k}) = 0 \tag{1.110}$$

Therefore

$$c_{2k+2} = \frac{(2k+l)^2 + 2(2k+l) - l^2 - \mu^2}{(2k+2)(2k+2l+2)}c_{2k} \tag{1.111}$$

The recursion relation (1.111) reduces to a polynomial of order n if

$$\mu^2 = n^2 + 2n - l^2 \tag{1.112a}$$

$$n = 2k + l \tag{1.112b}$$

(1.111) can be rewritten as

$$\begin{aligned} c_{2k} &= \prod_{i=1}^{m} \frac{(-1)i(n+1-i)}{(k+1-i)(n+1-k-i)} c_{2k-2m} \\ &= \frac{(-1)^k \Gamma(n+1)\Gamma(n+1-2k)}{\Gamma^2(n+1-k)} c_0 \end{aligned} \tag{1.113}$$

Choose

$$c_0 = \frac{1}{\Gamma(n+1)} \tag{1.114}$$

then

$$c_{2k} = \frac{(-1)^k \Gamma(n+1-2k)}{\Gamma^2(n+1-k)} \tag{1.115}$$

(1.112) gives the energy spectrum and $u(x)$ is the eigen function.

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Chapter 2

Classical Field Theory of Transport of Interacting Classical Particles Through One-dimensional Channels

Parallel to the study of low dimensional quantum systems, a number of molecular simulations have been carried out to understand water transport through one-dimensional channels. In this chapter, I explore the role of a dimensionality constraint on the collective excitations of a classical system in one dimension. I show the intrinsic connection between the classical field theory and the corresponding quantum theory, i. e. Tomonaga-Luttinger liquid thoery, which describes the interacting fermions in one dimension and the effective quantum field theory for the Bosonic systems developed in chapter 1. As applications, I calculate the particle density function along the tube axis and the particle current through the channels by explicitly including the particle-particle and particle-wall interactions. I find a quantum-classical correspondence in the conductance formula.

2.1 Introduction

Particle dynamics in one dimension (1D) is of great current interest, in both classical and the quantum mechanical regimes. In the latter case, the dimensionality constraint plays an extremely important role; due to the peculiar topology of the Fermi surface in 1D, strongly correlated electrons in 1D are described by the Tomonaga-Luttinger model [1, 2] rather than the usual Fermi liquid model. On the other hand, although there have been a number of important theoretical studies of the dynamics of classical particles, e. g. , water molecules and ions in one-dimensional channels [3, 4, 5, 6, 7], the role of the dimensionality constraint in such systems has not been considered in a fundamental manner. A comparison of and a possible unification of the classical and quantum theories of transport in one-dimensional mesoscopic channels is therefore of both theoretical and experimental interest.

Molecular dynamics studies of the motion of water molecules in hydrophobic and/or hydrophilic channels [3, 4] and proton transport in carbon nanotubes [5] have provided evidence for such striking phenomena as rapid transport, burst-like transmission, and particle density oscillations along the tube axis. Contrasting probabilistic models have been suggested to describe these effects: a random walk (CTRW) model [6] in which a chain of water molecules moves as a whole, and a single particle sequential hopping model without particle-particle correlation [7]. These contrasting views suggest the need for a microscopic theory that explicitly includes the particle-particle (PP) interactions as well as the particle-wall (PW) interactions.

In this work, we construct a classical field theory of interacting classical particles and dimensionality constraint. Its relation to the theory of interacting fermions in 1D (Refs. 1 and Refs. 8) is established at the Hamiltonian level. As applications, we obtain the particle density function (PDF) along the tube axis (the $\hat{z}$ direction) and an expression for the particle current, and compare with earlier results.

2.2 Theory

Generally in kinetic theory, the PW interaction is neglected and PP interactions are difficult to treat exactly in phase space, e. g., the Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy. However, the available phase space is severely restricted by the physical dimensionality, which makes some special models exactly solvable.

Consider a system of N particles of mass m, confined in a 1D channel of length L, subjected to periodic boundary conditions. Define a simple system by the following interactions: (1) hard-sphere exclusion; (2) elastic collisions. Such a simple system is equivalent to a system of free particles, if the following conditions hold: (i) spatial dimension $d = 1$; (ii) identical particles; (iii) $\Delta t > \tau_c$, $\Delta x > r_0$ where Δt, Δx are temporal, spatial resolutions and τ_c, r_0 are the collision time and the effective diameter of the particles, respectively. The proof is as follows:

(1) Collisions: For particles 1 and 2, let $p1$, $p2$ be the momenta before the collision and $p1'$, $p2'$ be the momenta after the collision. Since $d = 1$, collisions are head on collisions. Since collisions are elastic in a simple system, $p1' = p2$, $p2' = p1$. Since particles are identical, we can define a set of new particles or modes which propagate freely on the scales set by conditions (iii).

(2) No collisions: Each particle propagates freely.

The newly defined set of particles (or modes) for a simple system are many body in nature and they greatly simplify the problem by maximally utilizing the conservation of particles, as will become clear later. We will refer to this new set simply as particles or momentum (velocity) modes in the rest of this paper.

For N particles $\{x_n(t)\}$, the density of particles $\rho(x,t)$ and the current density $J(x,t)$ are

$$\rho(x,t) = \sum_n \delta(x - x_n(t)) \tag{2.1}$$

$$J(x,t) = \sum_n \frac{dx_n(t)}{dt}\delta(x - x_n(t)) \tag{2.2}$$

If the N particles are subjected to no external forces, the energy-momentum tensor $T^{\mu\nu}(t,x)$ in the non-relativistic regime is

$$T^{\mu\nu}(t,x) = \sum_n P_n^\mu(t)\delta(x - x_n(t))\frac{dX_n^\nu}{dt}, \quad \mu = 0, 1 \tag{2.3}$$

where

$$X_n^\nu \equiv (t, x_n(t)) \tag{2.4a}$$

$$P_n^\mu(t) \equiv (\varepsilon_n(t), p_n(t)) \tag{2.4b}$$

are defined as two-vectors and two-momenta, respectively, with

$$p_n(t) = m\frac{dx_n(t)}{dt} \tag{2.5a}$$

$$\varepsilon_n(t) = \frac{p_n^2(t)}{2m} \tag{2.5b}$$

For free particles, we have $\frac{dP_n^\mu(t)}{dt} = 0$. The conservation of the total energy and momentum can be expressed by the continuity equation satisfied by the energy-momentum tensor:

$$\partial_\nu T^{\mu\nu} = 0 \tag{2.6}$$

The $\mu = 1$ component of the Eq.(2.6) corresponds to the conservation of total momentum, which can be written in terms of $J(x,t)$ as

$$\partial_t J(x,t) = -\partial_x \sum_v \sum_{|u|=v} u^2 \sum_{n_u} \delta(x - x_{n_u}(t)) \tag{2.7}$$

where $n_u \in \{n|\frac{dx_n(t)}{dt} = u\}$. A summation on v is over all the velocity modes in the N-particle system. (Particles that propagate with $\pm v$, by definition, belong to the same velocity mode v.) The conservation of particles is the equation of motion of the particle density $\rho(x,t)$

$$\partial_t \rho(x,t) = -\partial_x J(x,t) \tag{2.8}$$

Define the dynamical field $\phi(x, t; v)$ and its conjugate momentum density $\pi(x, t; v)$ such that

$$\partial_x \phi(x, t; v) \equiv \rho_0 - \sum_{n_u, |u|=v} \delta(x - x_{n_u}(t)) = \rho_0 - \rho(x, t; v) \tag{2.9}$$

$$\pi(x, t; v) \equiv \frac{\hbar_v}{v} \sum_{n_u, |u|=v} u\delta(x - x_{n_u}(t)) \tag{2.10}$$

where ρ_0 is a constant which may be different for different models; however, the e.o.m. of $\phi(x, t; v)$ and $\pi(x, t; v)$ will not be changed by this constant. $\hbar_v$ has the dimension of action and it is a constant for each velocity mode v. We can obtain the e.o.m. of $\phi(x, t; v)$ and $\pi(x, t; v)$ immediately from Eqs. (2.7) and (4.47)

$$\partial_t \phi(x, t; v) = v\pi(x, t; v)/\hbar_v \tag{2.11}$$

$$\partial_t \pi(x, t; v) = \hbar_v v \partial_x^2 \pi(x, t; v)/\hbar_v \tag{2.12}$$

Up to a surface term and a constant, the noninteracting field Hamiltonian for the classical particles in 1D is obtained

$$H_0 = \sum_v \frac{\hbar_v v}{2} \int_0^L dx \{\pi^2(x; v)/\hbar_v^2 + [\partial_x \phi(x; v)]^2\} \tag{2.13}$$

In constructing the Hamiltonian (2.13), we employ the continuity equations of the conserved quantities: particles, energy, and momentum. It is worth pointing out that in 1D the conservation of particles is more fundamental than the other two due to the unique dimensional and geometric constraint. In addition, the defined free particles (momentum modes) facilitate the possibility to identify the density current Eq.(2.11)and the axial current Eq. (2.12) from the conservation of total particles Eq. (4.47), upon which we find the dynamical field $\phi(x, t; v)$ and its conjugate momentum density $\pi(x, t; v)$. Furthermore, the field Hamiltonian (2.13) is a general *structural* Hamiltonian, which is determined by the conservation laws and the 1D constraint, yet the definite physical meaning of the fields $\phi(x, t; v)$ and field parameters ρ_0 and $\hbar_v$ are still up to specific models.

By canonical quantization

$$[\phi(x;v),\pi(y;v)]=i\hbar\delta(x-y) \tag{2.14}$$

the Hamiltonian (2.13) is then a collection of massless free boson scalar fields. If only one of the velocity modes is important, which is the case for the electrons confined in 1D at the low energy regime, and upon velocity and field renormalization due to electron-electron interactions, the Tomonaga- Luttinger Hamiltonian [7, 9] is obtained. In fact, Dzyaloshinskii and Larkins solution [10] to the 1D interacting fermion problem using Ward identities also relies on the realization of the important role played by the conservation of charges (particles) in 1D: in the 1+1 dimensions, the conservation of axial charges (particles) together with total charges (particles) determine the low energy structure of theory. This is directly related to the 1D constraint (disconnected Fermi surface) [11].

The physical interpretation of the classical field Hamiltonian (2.13) and the origin of the various parameters: ρ_0, $\hbar_v$ can be made clear by considering the following 1D lattice model of $\mathcal{N}$ sites, with occupation number $n_i \in \{0,1\}$, $\forall i \in \mathcal{N}$. Without losing generality, examine a subset of all the particles which propagate with the same velocity $\pm v$. Define the dynamical variable $\tilde{\phi}_i$ to be

$$\tilde{\phi}_i \equiv -\sum_{j\leq i} n_j \tag{2.15}$$

For 1D geometry, it is convenient to separate the left (L) and the right (R) moving particles:

$$\phi_{i,L(R)} \equiv -\sum_{j\leq i} n_{j,L(R)}, \quad n_{j,L(R)} \in \{0,1\} \tag{2.16}$$

with the properties $n_{i,L}+n_{i,R}=n_i$ and $n_{i,L}n_{i,R}=0$. So the free part of the Hamiltonian can be written in terms of these left and right moving particles

$$H_{0,v}=mv^2a\sum_{i,r} a\left(\frac{n_{i,r}}{a}\right)\left(\frac{n_{i,r}}{a}\right)-\frac{mv^2}{2}\sum_{i} a\left(\frac{n_i}{a}\right) \tag{2.17}$$

where a is lattice spacing and $r = L, R$. The form of the lattice Hamiltonian is not unique at first glance; however, in 1D, since the structure of continuum limit Hamiltonian (2.13) is *determined* by conservation laws Eq. (2.7) and Eq. (4.47), the corresponding form of lattice Hamiltonian is restricted that of (2.17).

In the continuum limit:

$$\tilde{\phi}_i \rightarrow \tilde{\phi}(x;v) = -\int_0^x dy\rho(y;v) \tag{2.18}$$

$$\tilde{\phi}_{i,L(R)} \rightarrow \tilde{\phi}_{L(R)}(x;v) = -\int_0^x dy\rho_{L(R)}(y;v) \tag{2.19}$$

and the Hamiltonian (2.17) becomes

$$H_{0,v} \rightarrow \hbar_v v \int_0^L dx\{[\partial_x\phi_L(x;v)]^2 + [\partial_x\phi_R(x;v)]^2\} - E_0 \tag{2.20}$$

where $\hbar \equiv mva$ and

$$E_0 = -\frac{mv^2}{2}\int_0^L \partial_x\tilde{\phi}_L(x;v) \tag{2.21}$$

Defining the dynamical field $\phi(x;v)$ and its conjugate momentum density $\pi(x;v)$ by

$$\partial_x\phi(x;v) \equiv \partial_x\tilde{\phi}(x;v) + \rho_0 = -\rho(x;v) + \rho_0 \tag{2.22}$$

$$\begin{aligned} \pi(x;v) &\equiv \hbar_v[\rho_R(x;v) - \rho_L(x;v)] \\ &= -\hbar_v[\partial_x\phi_R(x;v) - \partial_x\phi_L(x;v)] \end{aligned} \tag{2.23}$$

with $\rho_0 = \frac{1}{2a} = \frac{\mathcal{N}}{2L}$, we obtain the field Hamiltonian:

$$H_{0,v} = \frac{\hbar_v v}{2}\int_0^L dx\left\{\frac{\pi(x;v)^2}{\hbar_v^2} + [\partial_x\phi(x;v)]^2\right\} \tag{2.24}$$

In this lattice model, ρ_0 is taken to be a uniform density of half a particle per site, so $-\partial_x\phi(x,t;v)$ is equivalent to a spin-$\frac{1}{2}$ density with $+1/2a$ spin up (site occupied) and $-1/2a$

spin down (site unoccupied). h_v is defined such that the definition of $\pi(x,t)$ Eq. (2.23) is consistent with the actual momentum density. A summation over all the velocity modes will then give the field Hamiltonian (2.13).

We now consider PP (besides the hard-sphere interaction) and PW interactions. The general form of the two-body PP interaction in 1D is

$$H_{PP} = \frac{1}{2}\int_0^L dxdyV_{PP}(x,y)\rho(x)\rho(y) = H_2 + H_4 \tag{2.25}$$

H_2 is the forward scattering between the left (L) and the right (R) branches, while H_4 is the forward scattering in the same branch. The PP interaction will generally couple the dynamics of individual *particles* and thus complicate the microscopic treatment of the transport. To simplify the theoretical description, a standard procedure would be finding the normal modes of the interaction. The many-body *velocity modes* defined above are the normal modes of the hard-sphere PP interaction. These normal modes renormalize only when there is also a nonlinear interaction, e.g., the soft part of the PP potential, which generates inelastic scattering processes. Obviously, these processes do not ensure a perfect gas approximation or an isentropic flow. The exact solution to the 1D imperfect and nonisentropic flow is a difficult task [10]. Nevertheless, we proceed to propose a simplified model based on the generic results observed in molecular dynamics simulations:[3, 6, 13](1) a threshold energy E_{th} k_BT exists for interacting particles to enter the 1D channel, so only a few activated modes are responsible for the transport; (2) interacting particles transport through a 1D channel is highly collective unhindered by the interactions with the walls. A concerted motion in the channel is observed; (3) the time series of the number of particles transported through a 1D channel falls into a narrow range 20/ns. These simulation results suggest a simplified two-parameter model: The first parameter v_0 is the typical velocity mode responsible for the transport through a 1D channel connecting to two fluid reservoirs. In fact, small perturbations to an equilibrium fluid would propagate with the velocity of sound, which are then transmitted into a 1D channel. The boundary conditions require the pressures and normal velocity components of the incident, reflected, and transmitted waves to be equal at the contact regions. The second parameter K describes the PP interaction within the mode v_0, which is described below. Even with these simplifications, we find the theory exhibits rich physical phenomena and qualitatively explained the results of the simulations.

In 1D and the continuum limit, the PP interaction can be taken to be local [14]; we therefore have

$$H_2 = -\frac{\hbar v_0 g_2}{2}\int_0^L dx\left[\frac{\pi^2}{\hbar^2} - (\partial_x\phi)^2\right] \tag{2.26}$$

$$H_4 = -\frac{\hbar v_0 g_4}{2}\int_0^L dx\left[\frac{\pi^2}{\hbar^2} + (\partial_x\phi)^2\right] \tag{2.27}$$

where $\hbar \equiv m v_0 a$, and $g_2 = g_4 = \frac{V_{pp}}{2mv_0^2}$ for density-density interactions but can be taken as parameters in a more general case. g_2 and g_4 are negative if the PP interaction is attractive and they are positive if the PP interaction is repulsive. The PP interaction renormalizes the velocity of the density wave and the fields.

In the nanoscale, the inhomogeneous PW interaction, which can arise either from the atomic structure of carbon nanotube wall or the complex composition of the cell membrane, etc., become important and cannot be neglected. The general form of the PW interaction is

$$H_{PW} = -\int_0^L dx V_{PW}(x)(\partial_x\phi) \tag{2.28}$$

where $V_{PW}(x)$ is equivalent to a spatial varying magnetic field. The total Hamiltonian is obtained

$$\begin{aligned} H &= \frac{\hbar v}{2}\int_0^L dx\left[\frac{K\pi^2}{\hbar^2} + \frac{1}{K}(\partial_x\phi)^2\right] - \int_0^L dx V_{PW}(x)(\partial_x\phi) \\ &= H_0 + H_{PP} + H_{PW} \end{aligned} \tag{2.29}$$

The renormalized density wave velocity

$$v = v_0\sqrt{(1+g_4)^2 - g_2^2} \tag{2.30}$$

The PP interaction parameter is

$$K = \sqrt{(1 - g_2 + g_4)/(1 + g_2 + g_4)} \tag{2.31}$$

with $K > 1$ for attractive PP interaction, $K < 1$ for repulsive PP interaction, and $K = 1$ for noninteracting particles. In the case of inhomogeneous interaction, v and K are spatial dependent.

The particle density along $\hat{z}$ direction is obtained by solving the canonical e.o.m. of the field $\phi(x, t)$:

$$\partial_t^2 \phi = v^2 \partial_x^2 \phi + \frac{vK}{\hbar} \frac{dV_{PW}}{dx} \tag{2.32}$$

subject to periodic boundary condition and initial conditions. The contribution from initial conditions are time averaged to zero and the steady PDF is

$$\rho(x) = \rho_0 - \frac{KV_{PW}(x)}{\hbar v} = \bar{\rho} + \rho_s(x) \tag{2.33}$$

The average particle density $\bar{\rho}$ and the variation density $\rho_s(x)$ due to channel structure are

$$\bar{\rho} = \rho_0 \left(1 - \frac{2\bar{V}_{PW}}{V_{PP} + mv_0^2}\right) \tag{2.34}$$

$$\rho_s(x) = -\frac{2\bar{V}_{PW}^{(s)}(x)\rho_0}{V_{PP} + mv_0^2} \tag{2.35}$$

where

$$\bar{V}_{PW} = \frac{1}{L} \int_0^L dx V_{PW}(x) \tag{2.36}$$

is the average PW interaction. $V_{PW}^{(s)}(x) = V_{PW}(x) - \bar{V}_{PW}$ is the inhomogeneous part of the PW interaction and it is directly related to the wall structure. The intrinsic parameter ρ_0 of the field theory appeared in the density function $\rho(x)$ can be scaled away by defining the corresponding density $\rho_r(x) \equiv \rho(x)/\bar{\rho}$

$$\rho_r(x) = 1 - \frac{2\bar{V}^{(s)}_{PW}(x)}{(V_{PP} - 2\bar{V}_{PW}) + mv_0^2} \tag{2.37}$$

which is a good observable. We find (1) the structure of the PDFs (2.35) and (2.37) is determined by the channel wall structure and composition. We identify the particle density oscillation periodicity observed in [3] and Fig. 3 (2.6$\AA$) of [4] as the periodicity of the atomic lattice wall. (2) If the 1D channel is connected to reservoirs, the average particle density (2.34) is determined not only by the PW coupling strength but also by the PP interaction and the particle kinetic energy. Note that the change of particle density due to PW interaction modification is more sensitive for the attractive PP interaction than for the repulsive PP interaction.

The particle current through the 1D channel is directly related to the dynamics of the field $\phi(x, t)$

$$J(x,t) = \frac{v_0 \pi(x,t)}{\hbar} = \partial_t \phi(x,t) \tag{2.38}$$

Consider an external driving field $U_{ex}(x,t) = e^{-i\omega t}U(x) + c.c.$ coupled to the system. The corresponding interaction Hamiltonian is

$$H_{int} = -\int_0^L dx U_{ex}(x,t)\partial_x \phi \tag{2.39}$$

The contact regions are included as part of the 1D channel. In the limit of $\omega \rightarrow 0$, the steady state current is obtained

$$J(x) = \lim_{t\to\infty}\langle J(x,t)\rangle = \frac{K(\Delta U_{ex} + \Delta V_{PW})}{2\hbar} \tag{2.40}$$

where the time average is taken. ΔU_{ex} and ΔV_{PW} are the difference in the external potential and PW interaction between the two contact regions. If the current is caused by the pressure difference, then $\Delta U_{ex} = \mu_L - \mu_R$, where $\mu_{L/R}$ is the chemical potential of the left and/or right reservoir. The hydraulic permeability L_P is

$$L_P = \frac{J(x)}{\Delta P} = \frac{K}{2mv_0r_0}\left(\frac{\partial\Delta\mu}{\partial P}\right)_T \qquad (2.41)$$

The expression of the current (2.40) is the same as that of the electric current for a quantum wire, except that for the classical particle current, $\hbar$ depends on lattice spacing (we take $a \sim r_0$) and the bare density wave velocity. The current and hydraulic permeability explicitly depend on the PP interaction, with higher current for the attractive PP interaction ($K > 1$) and lower current for the repulsive PP interaction ($K < 1$). In this model, the steady state current does not depend on the detailed PW interaction or the length of the channel. This is in agreement with the molecular dynamics [13, 15] and experimental [16] results. However, if the PW attractive interaction dominates over kinetic energy, then an activated sequential transport theory is needed and the current will depend on the PW interaction strength and channel length.

2.3 Future Direction and Conclusions

Extensions of our model to structured particles can be made straightforwardly. For example, water molecules with dipolar orientation can be mapped to electrons with spins. The classical theory will correspond to the TL liquid theory with spin degree of freedom, where spin-charge separation was predicted. Though the Umklapp backscattering is not present in the classical model, the hydraulic permeability (2.41) is determined by the interaction parameter K resembling the quantum case. If reservoirs together with the 1D channel are modeled as an inhomogeneous system as a whole, the permeability would be determined by the interaction parameters of the reservoirs instead. So it would be interesting to study classically how sound waves of reservoirs are transmitted and reflected at the exits and/or entrances in the presence of interactions. In particular, what is the classical mechanism of the transformation from the many-body reservoir modes to those of the 1D channel as compared to the quantum case [17, 18]; what are the functional structures in biological 1D systems that facilitate the transformation. On the other hand, the effects of classical PP interaction, repulsive or attractive (e.g., hydrogen bonding), on particle current could provide an interesting insight into the effects of electron-electron interaction on electric conductivity in 1D. In addition to the above extensions, we note that a general solution of one dimensional isentropic flow is given by Landau and Lifshitz12 in terms of a linear differential equation valid for imperfect and perfect gases but only easily solvable in the latter case. It would be interesting to compare our results including particle-particle interactions with those of the treatment of Landau and Lifshitz[10]. This will be considered in a subsequent paper.

In conclusion, we have constructed a classical field theory for interacting classical particles (structureless) in 1D channels. The unification of the classical and quantum theories is a direct consequence of the 1D dimensionality constraint and the conservation laws. Because of these constraints, the density wave and/or particle-hole excitation is generic for particle-conserved systems in 1D. In our simplified model, the field theoretical calculations showed that both PW and PP interactions are important to the filling process, while PP interaction determines the steady state transport properties. We hope the simplified model will serve as a basis for extension to more complicated situations.

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Chapter 3

Fluorescence Intermittency of A Single Quantum System and Anderson Localization

From this chapter on, I will study how a single system responses to a complex environment, where the complex dynamics of the environment cannot be easily studied through first principles. Therefore, disorder and stochastic processes are necessary for studying this type of systems. In this chapter I consider the quantum regime and propose a model in which a quantum system is embedded in a complex and non-ergodic environment. I will show that the statistics of photon emissions from this single quantum system contains the information of the disordered environment. By applying our model to the fluorescence intermittency of semiconductor quantum dots (QD) and single molecules (SM), I show this can be understood from the thoery of Anderson localization. The power law distribution for the *on* time is explained as due to the interaction between QD/SM with a random environment. In particular, we find that the *on*-time probability distribution behaves differently in the localized and delocalized regimes. They, when properly scaled, are *universal* for different QD/SM systems. The *on*-time probability distribution function in the delocalized QD/SM regime can be approximated by power laws with exponents covering $-2 \leq m < 0$. Part of this work is published in *cond-mat/0601092*

3.1 Introduction

Recent developments in nano-fabrication and measurement have made it possible to probe directly the dynamics of a single quantum system and its coupling with its local environment. For optical measurements, in particular, fluorescence intermittency (FI) occurs in a wide class of single quantum systems including semiconductor nanocrystals [1, 2, 3, 4, 5] and single molecules [6, 7, 8]. This optical phenomenon is experimentally found to be a robust and fundamental property of single photon emitters. The random switching between an emitting (*on*) and a non-emitting (*off*) state is characterized by *on*-time and *off*-time distribution functions. Surprisingly, the distribution functions can often be fitted by power laws instead of exponentials. The exponents of the power laws vary from system to system and they are almost independent of temperature. To explain this unusual behavior, Marcus *et. al.* [9, 10] recently proposed a model based on diffusion in energy space. An exponent of -1.5 is readily obtained for one-dimensional diffusion processes. Deviation from -1.5 is explained by anomalous diffusion, which has its origin from the Cole-Davison dielectric medium $\beta \neq 1$. However, this scenario would predict exponents that are temperature dependent. Recent experiments also found that exponents ~ -2.0 for the *on* time occur in many different single emitters [1, 4, 6, 7, 8], which are imbedded in various media. The temperature-independence of power laws with $m_{\text{on/off}} \neq -1.5$ and robustness of $m_{\text{on}} = -2.0$ need to be explained.

In this work, we provide a microscopic Hamiltonian model which does not build on the assumption of anomalous diffusion in energy space and the quadratic form of diffusion potential. The purpose of this work is to lay the foundation for a quantum-mechanical theory of FI. In a classic paper [11], Anderson considered a transport process which involves solely quantum-mechanical motion in a random lattice. His quantum-mechanical treatment of the process leads to the concept of Anderson localization, which has been applied extensively to the problem of transport in a random environment. Here, we view the blinking as a charge hopping process between the QD/SM and the traps in the environment. We find that the

FI can be explained in the framework of the Anderson localization. The basic idea is the following: due to the coupling to a random environment, the on-site energy of a QD/SM is renormalized and becomes a random variable. In addition, random configurations of the local environment lead to a distribution of decaying (hopping) rates for the QD/SM. This is the physical origin of the *on*-time distribution.

3.2 Theory

Based on experimental results, we study the following simple tight-binding Hamiltonian:

$$\hat{H} = \varepsilon_d \hat{d}^\dagger \hat{d} + \sum_j \varepsilon_j \hat{c}_j^\dagger \hat{c}_j + \sum_j v_j \left(\hat{d}^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{d} \right) \tag{3.1}$$

The ground state is defined such that the QD/SM is neutral. For a QD this corresponds to a filled valence band. When an electron is excited by photon to an excited state, it relaxes to the lowest excited state on a time scale from hundreds of femtoseconds to picoseconds. This lowest excited state is responsible for photon emission and hopping to traps in the matrix. This state could be $1S$ state for QDs and it may involve some surface states as well [12, 13]. The excited electron completes a radiative cycle on a time scale of the order inverse Rabi frequency: $\Omega_{\text{Rabi}}^{-1}$. This time scale is much smaller than the typical bin size, $\geq$0.2 ms, used in the experiments. Since the excited electronic state is near resonance with the ground state plus a photon, we define the *on*-state as the following: it is a dressed electronic state [14] which has the same bare energy as the excited electronic state, ε_d, but with an infinite lifetime when it is decoupled from the trap states. Physically, this means that when there is no coupling to the environment, the excited electron localizes inside the QD/SM and the QD/SM, being in the *on*-state, keeps emitting photons. Such an *on*-state is created by operator $\hat{d}^\dagger$. The bare on-site energy ε_d is renormalized due to interaction with trap sites j. The coupling constant is v_j. The trap site j is created by operator $\hat{c}_j^\dagger$ and has a random energy ε_j. Here we focus on the class of random environments that are formed by a topologically random network of chemical bonds. Randomness could arise from a spatially fluctuating potential due to charged impurities and coupling with phonons that arise from deformation of a random lattice. The details of randomness are irrelevant to the dynamical response of the system as is known from scaling theory of localization. For simplicity, we assume all traps follow the same energy distribution function $p(\varepsilon)$.

Mathematically, the above definitions are equivalent to defining the zeroth order Green's function of the *on*-state as:

$$G_d^{(0)}(\omega) = \frac{1}{\omega - \omega_d + i\eta} \tag{3.2}$$

with $\omega_d = \varepsilon_d/\hbar$, and η being an infinitesimally small and positive constant. Similarly, the zeroth order Green's functions of the traps are

$$G_j^{(0)}(\omega) = \frac{1}{\omega - \omega_j + i\eta} \tag{3.3}$$

The decay rate of the *on*-state can be calculated from the full Green's function

$$G_d(\omega) = \frac{1}{\omega - \omega_d - \Sigma_s(\omega)} \tag{3.4}$$

where the only self-energy of the model is

$$\Sigma_s(\omega) = \frac{1}{\hbar^2}\sum_j \frac{v_j^2}{\omega - \omega_j + i\eta} \tag{3.5}$$

One obtains the renormalized energy and decay rate from the pole equation. The results to $O(v_j^2)$ are:

$$E_d = \varepsilon_d + \sum_j \frac{v_j^2(\varepsilon_d - \varepsilon_j)}{(\varepsilon_d - \varepsilon_j)^2 + \eta^2} \tag{3.6a}$$

$$\Gamma = \sum_j \frac{2v_j^2}{\hbar}\frac{\eta}{(\varepsilon_d - \varepsilon_j)^2 + \eta^2} \tag{3.6b}$$

Since each ε_j is a random variable, both the renormalized energy E_d and decay rate Γ are random variables. Physically, this corresponds to the situation in which environment stays at a certain configuration for a period of time during which a physical decay rate can be defined.

The ensemble of configurations that the environment takes on gives rise to a distribution of decay rates. This picture is valid when static disorder dominates or when the environment is ergodic.

To find the decay rate distribution function, $f(\Gamma)$, from $p(\varepsilon_j)$, one must perform a summation over random variables ε_j. In addition, due to lattice deformation, a random spatial distribution of traps must also be assumed. For simplicity, we assume that all the traps follow the same distribution function $\rho(\mathbf{r})$. We will consider two physical regimes, namely the delocalized and the localized regimes, for the excited electron on the QD/SM according to the framework of Anderson [11].

The delocalized regime corresponds to most of the experimentally studied situations. Essentially, electrons excited inside the QD/SM can make real transitions to the trap sites in the matrix through the mechanism of quantum tunneling, and then become localized. When this happens, the QD/SM becomes ionized. The results in this regime, which will be shown later, support the random resonance picture: on average, the energy of a QD/SM, is far off-resonance with the trap energies, i.e. $\varepsilon_d \gg \varepsilon_j$. The electrons of QD/SM remain localized (*on* state) until a random fluctuation of ε_j makes it on-resonance with the QD/SM. This random resonance could be realized through interaction with phonons [17]. Since there is finite probability that $\varepsilon_d - \varepsilon_j \sim \eta \sim 0^+$, one cannot perform the summations in the same way as in [11]. Instead, nontrivial summations of the whole expression (3.6b) are required. The distribution function $f(\Gamma)$ can be calculated by method of Fourier transformation:

$$f(\Gamma) = \int_{-\infty}^{\infty} \frac{dt}{2\pi}\, \psi(t)\, e^{-i\Gamma t} \tag{3.7}$$

The Fourier transformed probability distribution function $\psi(t)$ is given by

$$\begin{aligned} \psi(t) &= \int_{-\infty}^{\infty} \prod_{j=1}^{N} d\varepsilon_j p(\varepsilon_j) \exp\left[it \sum_{k=1}^{N} \frac{2v_k^2}{\hbar} \frac{\eta}{(\varepsilon_d - \varepsilon_k)^2 + \eta^2} \right] \\ &= \exp\{N \ln \mathcal{I}\} \end{aligned} \tag{3.8}$$

where N is the number of traps and

$$\mathcal{I} = \int_{-\infty}^{\infty} d\varepsilon \int d\mathbf{r}\; p(\varepsilon)\rho(\mathbf{r}) \exp\left[i \frac{2tv(\mathbf{r})^2}{\hbar} \frac{\eta}{(\varepsilon_d - \varepsilon)^2 + \eta^2} \right]$$

The integral $\mathcal{I}$ is obtained under the assumptions made above, i.e. identical energy and spatial distributions of traps. This integral needs to be done carefully so that we can express it in powers of η. For a real physical system coupled to a disordered environment, η is small but nonetheless not strictly zero. Physically, this is due to competing non-radiative relaxation channels which contribute to a small but finite width of resonance. The value of η can be calculated in a more sophisticated model, however, in our model we take it as a fitting parameter. Changing variable to the dimensionless

$$u = \frac{\hbar}{2\pi v(\mathbf{r})^2 |t|} \varepsilon \tag{3.9}$$

and noticing $\frac{1}{\pi} \frac{\eta}{(u-u_d)^2+\eta^2}$ can be approximated by an impulse function centered at $u = u_d$ as η is sufficiently small, where

$$u_d = \frac{\hbar}{2\pi v(\mathbf{r})^2 |t|} \varepsilon_d \tag{3.10}$$

we can separate the integral into three parts: $(-\infty, u_d - \eta/2]$, $(u_d - \eta/2, u_d + \eta/2)$ and $[u_d + \eta/2, +\infty)$ to obtain the expansion:

$$\mathcal{I} = 1 - \eta \left[1 - \cos\left(\frac{1}{\eta}\right) - i\, \mathrm{sign}(t) \sin\left(\frac{1}{\eta}\right) \right] p(\varepsilon_d) \frac{2\pi}{\hbar} \langle v(\mathbf{r})^2 \rangle |t| + O(\eta^3)$$

Since we are interested in case where there are a large number of traps $N \gg 1$, by substituting the expansion into Eq.(3.8) we rewrite the unknown parameter $N\eta$ as $N\eta = a_0 n$ [11, 18], where n is the density of traps and a_0 is a fitting parameter. Absorbing the numerical constant in the square bracket of $\mathcal{I}$ into a_0 and neglecting an unimportant imaginary part as is justified in this delocalized regime, we get

$$\psi(t) = \exp\left\{ -\frac{2\pi}{\hbar} \langle v(\mathbf{r})^2 \rangle p(\varepsilon_d) n a_0 |t| \right\} \tag{3.11}$$

The probability distribution function $f(\Gamma)$ in the delocalized QD/SM regime:

$$f(\Gamma) = \frac{1}{\pi}\frac{\Gamma_0}{\Gamma^2 + \Gamma_0^2} \tag{3.12}$$

is Lorentzian, with the characteristic decay rate Γ_0 given by:

$$\Gamma_0 = \frac{2\pi}{\hbar}\langle v(\mathbf{r})^2\rangle p(\varepsilon_d) n a_0 \tag{3.13}$$

The *on*-time distribution function can be calculated as

$$P_{\text{on}}(t) = \int_0^\infty d\Gamma \exp(-\Gamma t) f(\Gamma) \tag{3.14}$$

which turns out to be:

$$P_{\text{on}}(t) = -\frac{2\Gamma_0}{\pi}\left[\cos(\Gamma_0 t)\text{ci}(\Gamma_0 t) + \sin(\Gamma_0 t)\text{si}(\Gamma_0 t)\right] \tag{3.15}$$

where ci and si are cosine and sine integrals [19] respectively.

The expression for $P_{\text{on}}(t)$ in (3.15) has several physical implications. First of all, it depends only on one parameter Γ_0 (this is also true for $P_{\text{on}}(t)$ in the localized regime (3.19), which only depends on the parameter γ_0). The characteristic decay rate Γ_0, is purely due to quantum tunneling and depends on the degree of disorder $p(\varepsilon_d)\langle v(\mathbf{r})^2\rangle$. This is a generic feature of Anderson localization theory. Only the energy fluctuation of traps evaluated at the bare QD/SM on-site energy, $p(\varepsilon_d)$, comes into the final result. This supports the random resonance picture discussed above. The one-parameter theory also implies that experimental results for different QD/SM systems, when plotted in unit of characteristic *on*-time lifetime $t_0 = 1/\Gamma_0$, follow a *universal* distribution Fig.3-1, Fig.3-2 and Fig.3-3. In the long time limit, $t \gg t_0$, $P_{\text{on}}(t) \sim t^{-2}$. The exponent of -2 comes from the peak of the Lorentzian distribution for decay rates, which physically indicates the resonant scattering condition. This -2 exponent is also robust and it does not depend on the properties of matrix or emitters [6]. In experiments, the observation time is fixed so that one probes only a certain

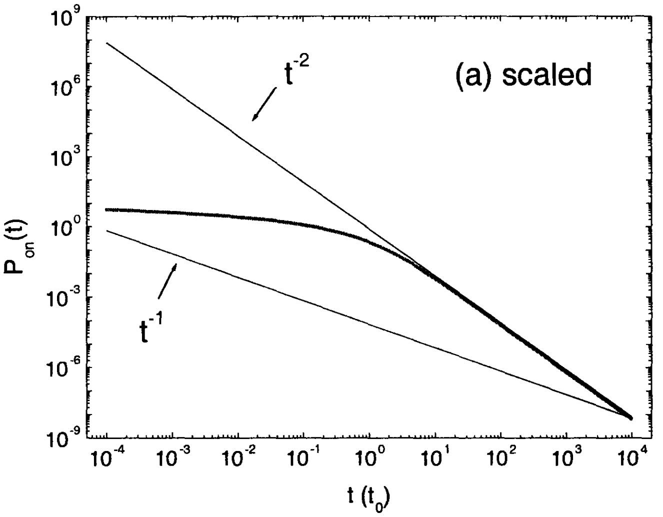

Figure 3-1: Probability distribution functions for the *on* time in the delocalized regime. Universal *on*-time probability distribution function obtained by scaling in a characteristic *on*-state lifetime $t_0 = 1/\Gamma_0$.

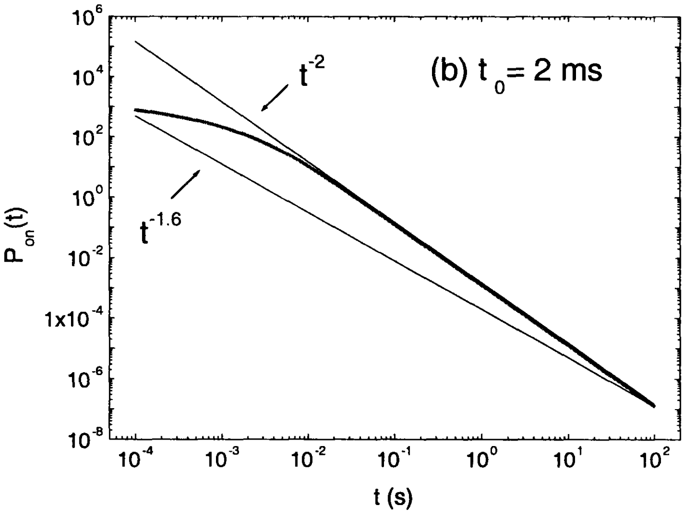

Figure 3-2: Probability distribution functions for the *on* time in the delocalized regime. $P_{\text{on}}(t)$ for a QD/SM with a lifetime 2ms and a fixed observation window. The exponents of the fitting power laws lie between -1.6 and -2.

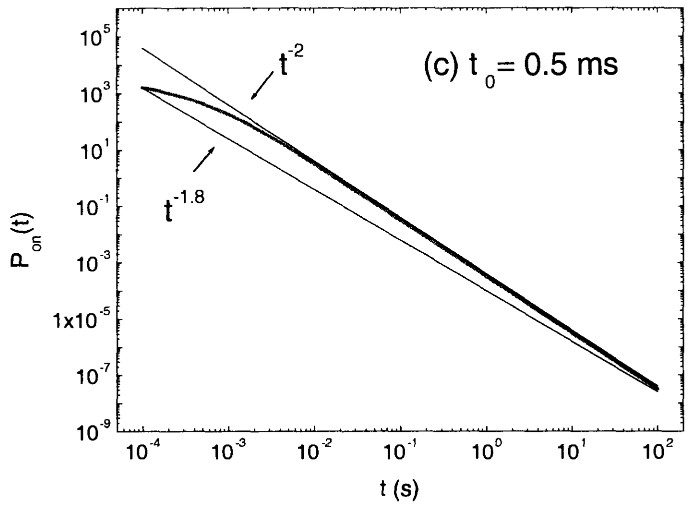

Figure 3-3: Probability distribution functions for the *on* time in the delocalized regime. $P_{\rm on}(t)$ of a QD/SM with a shorter lifetime 0.5ms. The exponents of the fitting power laws lie between -1.8 and -2.

range (3 to 4 orders of magnitude in physical time) of the whole probability distribution. The location of the window in the universal distribution depends on Γ_0, which is *not* universal. If one fits the experimental data with power laws, then the exponents of the power laws will implicitly depend on Γ_0 except for the $m_{\rm on} = -2$ case. From (3.13) we see that Γ_0 depends on properties of the QD/SM and its embedding matrix. This is one major difference between our theory and the diffusion-controlled electron transfer theory [9] for the *on*-time statistics. In the latter, the exponents of the fitting power laws come from properties of the dielectric medium alone, i.e. the β parameter of the Cole-Davison equation, which depends on temperature. As Γ_0 rises with increasing coupling strength between the QD/SM and its local environment, power law exponents observed for SMs would in principle larger than (in absolute value) that of well-coated QDs. This is indeed consistent with current experimental results[2, 6].

The quantum mechanical theory of FI allows a weak temperature-dependence of the *on*-

time probability density. This comes from the fact that the energy fluctuation of trap sites, besides the mechanisms discussed above, has a temperature component. This dependence is usually very weak since the typical energy difference between ε_d and ε_j is on the order of 1 $\sim$ 2 eV which is much larger than the magnitude of thermal broadening around ε_j. Increasing temperature slightly increases $p(\varepsilon_d)$ since $\varepsilon_d \gg \varepsilon_j$ and as a result Γ_0 increases. So higher temperature would slightly decrease m_{on} towards -2 for the long time.

In the case that the excited QD/SM electron is localized, then we predict very long *on* times. This corresponds to the off-resonance situation, $\varepsilon_d - \varepsilon_j \gg \eta, \forall j$. One can calculate the probability distribution of

$$\Gamma = \frac{2\eta}{\hbar} \sum_j \frac{v_j^2}{(\varepsilon_d - \varepsilon_j)^2} \tag{3.16}$$

using the results of [11]:

$$f(\Gamma) = \gamma_0^{\frac{1}{2}} \Gamma^{-\frac{3}{2}} \exp\left(-\pi\gamma_0/\Gamma\right) \tag{3.17}$$

where the characteristic decay rate γ_0 is

$$\gamma_0 = \frac{2\eta}{\hbar} \left[\frac{a_0 n \langle v(\mathbf{r})\rangle}{W}\right]^2 \tag{3.18}$$

W is the width of energy fluctuation for the traps. n is the density of traps, while $a_0 \sim O(1)$ is a constant with a dimension of volume. Note that in the limit $\eta \to 0$, then $\gamma_0 \to 0$ and the probability distribution function of decay rates is only nonzero when $\Gamma = 0$, i. e. the QD/SM electron is localized. Physically, the smallness of η has to be compared with the energy difference $\epsilon_d - \epsilon_j$ [15]. As discussed in the delocalized regime, the coupling of trap electrons with phonons and non-radiative processes etc. can lead to a sufficiently small, but non-zero value of η. The above results are applicable to many topologically disordered systems [16]. Thus, for a QD/SM in this regime, the single emitter experiences very long bright periods, which are characterized by $1/\gamma_0$. The *on*-time probability distribution function is obtained from (3.17):

$$P_{\text{on}}(t) = \left(\frac{t}{\pi\gamma_0}\right)^{-\frac{1}{2}} \exp\left(-\sqrt{4\pi\gamma_0 t}\right) \tag{3.19}$$

So in the limit $t \ll 1/\gamma_0$, the probability distribution of the *on*-time follows a power law with an exponent of $-1/2$. On a much longer time scale, $P_{\mathrm{on}}(t)$ deviates from the power law and shows a stretched-exponential tail. This stretched-exponential tail is of purely quantum nature and depends on the degree of disorder $W/\langle v(\mathrm{r})\rangle$.

Now we discuss the mechanism for the *off*-time probability distribution. Suppose a charge is on the trap site j. The self-energy of $G_j(\omega)$ is $G_d(\omega)$. The decay rate is vanishingly small, so the charge is localized. Then *on*-state can only be recovered via quantum tunnelling of trapped electrons. $P_{\mathrm{off}}(t)$ is therefore given by

$$P_{\mathrm{off}}(t) = \int_0^\infty dr g(r)\gamma_{\mathrm{off}}(r) \exp\left[-\gamma_{\mathrm{off}}(r)t\right] \tag{3.20}$$

where $g(r)$ is the probability density of an excited electron having been trapped at a distance of r from the QD/SM and it is proportional to the square of the excited state wave function. $\gamma_{\mathrm{off}}(r)$ is the decay rate of a trapped electron to the QD/SM. A model based on this picture was first proposed by Verberk *et.al.* [3] and experimentally examined in [5]. Since the typical size of a QD/SM is of the order 30Å in radius, so to a good approximation, the QD/SM can be viewed as a shallow impurity [20] and one can use effective mass theory. The wave function of an excited QD/SM electron behaves as $\exp(-r/a)$ at large distances, where

$$a = \frac{\hbar^2 \epsilon_0 \kappa}{m_d^* e^2} = \tilde{a}\kappa \tag{3.21}$$

is the effective Bohr radius and is related to the ionization energy, E_{ion}, of the excited electron by

$$a = \frac{\hbar}{\sqrt{2m_d^* E_{\mathrm{ion}}}} \tag{3.22}$$

κ is the relative static dielectric constants of the media. m_d^* is the effective mass of the QD/SM electron. Similarly, $\gamma_{\mathrm{off}}(r)$ is given by [17]:

$$\gamma_{\mathrm{off}}(r) = \gamma_{\mathrm{off}} \exp(-2r/b) \tag{3.23}$$

where $b = \hbar/\sqrt{2m_t^* E_t}$ is the spatial extent of a trapped electron's wave function with m_t^* and E_t being the effective mass and ionization energy at the trap site. We obtain

$$P_{\text{off}}(t) \approx C t^{-m_{\text{off}}} \tag{3.24}$$

with

$$C = \frac{a\Gamma(1 + b/a)}{b\ \gamma_{\text{off}}^{b/a}} \tag{3.25a}$$

$$m_{\text{off}} = 1 + \frac{b}{a} = 1 + \sqrt{\frac{m_d^* E_{\text{ion}}}{m_t^* E_t}} = 1 + \frac{b}{\tilde{a}} \frac{1}{\kappa} \tag{3.25b}$$

We see that the difference in m_{off} for different systems comes mainly from the effective mass m_d^* and the ability of a matrix to stabilize the charged QD/SM and the ejected electron. In contrast to the diffusion model [9], the exponents of $P_{\text{off}}(t)$ depend on the relative static dielectric constant κ instead of the Cole-Davison β parameter. This is consistent with recent experimental results [6, 5]. In addition, our model allows m_{off} to take a different value from m_{on} [1, 4, 6, 7], while the diffusion model predicts that they must be the same.

3.3 Conclusions

To conclude, we have proposed a mechanism for FI as being a manifestation of Anderson localization. The *on*-time manifold is shown to be generated by different realizations of electron delocalization from the QD/SM through the mechanism of random resonance. The quantum theory predicts a universal probability distribution function for the *on* time and shows $m_{\text{on}} = -2$ is indeed a robust result, which corresponds to the long time limit of $P_{\text{on}}(t)$. The *off* state corresponds to a localized electron in the environment. The recovery of the *on* state is realized via quantum tunneling.

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Chapter 4

Fluctuation and Its Propagation in Gene Networks

From the statistical mechanics point of view, the fluctuations of a system become negligibly small with increasing system size. The most probable configuration dominates over all other configurations. When the size of the system is very small, the fluctuations of an open system can be very large and thus completely change the deterministic picture. The fluctuations can arise from two sources: (1) External noise. The external noise comes from the coupling with the environment; (2) Internal or intrinsic noise. In contrast to the external noise, which can be controlled, the internal noise cannot simply be eliminated or reduced. In fact, the intrinsic noise can originate from spatial inhomogeneity, scattering anisotropy etc. As expected, the internal noise grows with decreasing size of the system. One challenge to the understanding of mesoscopic systems is to adequately incorporate fluctuations into theories. In these last two chapters, I will consider the fluctuations in the classical regime, e. g. biological systems, and consider its role in the properties and decision making of these important systems. In this chapter I consider molecule number fluctuation in a gene network. Based on the master equation, I will systematically derive various approximate approaches to this problem. In appendix, I provide a simple example of the simulation of a self-regulated gene network.

4.1 Introduction

In a deterministic picture, genetically identical cells exposed to the same environmental conditions should exhibit the same characteristics. However, this picture is not true on the molecular level. Stochasticity arises from fluctuations in transcription and translation even as the environment stays in constant conditions, and shows up as significant variation in molecular content and marked differences in phenotypic characteristics [1]. The process of gene expression involves several processes such as binding to the promoter, mRNA and protein synthesis and degradation, dimerization etc. all of which result from random encounters of two or more molecules. In large systems these processes can be simply written as rate equations such as:

$$A + B \underset{k_b}{\overset{k_f}{\rightleftharpoons}} P \tag{4.1}$$

where the change of concentration of product is

$$\frac{d[P]}{dt} = k_f[A][B] - k_b[P] \tag{4.2}$$

However in a small live cell, the fluctuation of molecule number is beyond the predictability of this deterministic rate equation. This fluctuation has both negative and positive consequences: It can have detrimental effects on cellular function with potential implications for disease. On the other hand, it can provide flexibility needed by cells to adapt to fluctuating environments or respond to sudden stresses. Studies have shown that regulatory gene networks exist in cells, that regulate the magnitude of molecule number fluctuations [2, 3, 4]. Quantitative analysis of these naturally occurring systems is often very difficult, thus the majority of experimental studies are directed to synthetic networks [5, 6, 7]. Both negative and positive feedback gene networks are studied. While in negative feedback gene networks, the molecule number distribution has one peak and is stable, the positive feedback gene network has a pronounced feature of bistability. In addition, gene cascade networks are studied where noise attenuation is observed. Most of the theoretical modelling for these experiments are based on Langevin equations generally of the form:

$$\frac{dx}{dt} = f(x) + \xi(x,t) \tag{4.3}$$

where gaussian white noise is usually assumed:

$$\langle \xi(x,t) \rangle = 0 \tag{4.4a}$$

$$\langle \xi(x,t)\xi(y,t') \rangle = g(x)\delta(x-y)\delta(t-t') \tag{4.4b}$$

However, the phenomenological Langevin equations are subject to criticism when $f(x)$ is nonlinear:

$$\frac{d\langle x(t) \rangle}{dt} = \langle f(x(t)) \rangle \neq f(\langle x(t) \rangle) \tag{4.5}$$

Thus fluctuations around a macroscopic solution must be studied in a more fundamental way.

In this chapter, I theoretically study a generic gene cascade network, based on which I study different ways of modelling this complex system. In particular, I study how noise propagates through the cascade as the length of the cascade increases.

4.2 One Dimensional Chain Model

To study how molecular number fluctuation propagates through a gene network, we design a one dimensional chain model as shown in figure 4-1. This gene network consists of N genes, each of which is represented as a box. Each gene synthesizes proteins which can regulate its

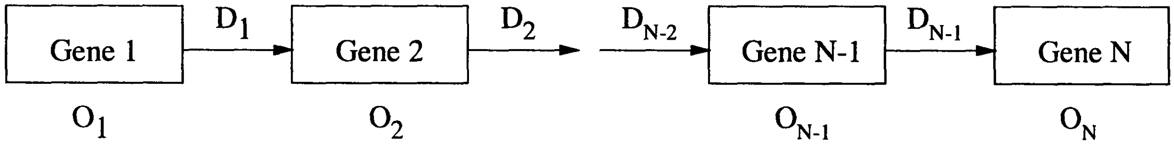

Figure 4-1: One Dimensional Chain Model

nearest downstream gene by mechanisms such as binding to a downstream operator. The status of each gene i is modeled as a two-state random variable $O_i \in \{\alpha, \beta\}$. This resembles a one dimensional Ising model. When a gene i is active, i. e. $O_i = \alpha$, it synthesizes proteins D_i (gene i is transcribed and the mRNA is translated). The proteins D_i can undertake several processes such as dimerization, degradation, and regulating a downstream gene. When a gene i is passive, i. e. $O_i = \beta$, the gene is not expressed and therefore no proteins are synthesized. The existing protein D_i can only be consumed by dimerization or binding to a downstream operator.

The transition dynamics

$$\alpha_i \rightleftharpoons \beta_i \tag{4.6}$$

is controlled by the nearest upstream protein D_{i-1} therefore a gene cascade is formed. See figure 4-2.

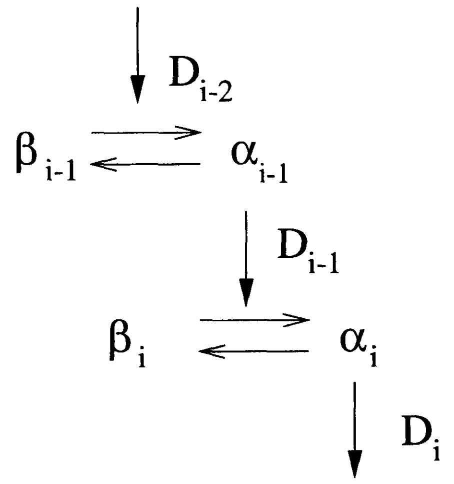

Figure 4-2: Regulation and Gene Cascade

4.3 Stochastic Modelling

The dynamics of the gene network constructed in the last section is studied phenomenologically in this section. No rigorous justification is given on this level of description and all processes are given as a result of plausible conjecture.

4.3.1 Protein Synthesis

The process of protein synthesis is one of the most complicated processes in a real gene network. It starts as unfolding of DNA, followed by processes such as transcription, ribosome binding, translation and dimerization etc. A complete description is beyond a single equation, however, if one is content with a relative large time scale, these processes can be summarized into a single stochastic differential equation:

$$dD_i(t) = -\Gamma_i(D_i)dt + k_i(t)dt + \tilde{\sigma}_i(D_i, t)dZ_t \tag{4.7}$$

where $D_i(t)$ is the number of proteins (dimer form) at time t.The first term in eq.(4.7) describes the consumption of protein, which includes

(a) protein degradation: $\gamma_i D_i$, where γ_i is a rate constant;

(b) binding to a downstream operator O_{i+1}: $\lambda_{i+1} f(D_i) n(O_{i+1})$, where λ_{i+1} is a rate constant, $f(D_i)$ is a binding function. Since the number of proteins is usually much larger than the number of downstream operators, we can neglect this process in the dynamics of protein.

The second term describes protein production with a time-dependent rate $k_i(t)$. Since protein production involves several processes, $k_i(t)$ is a mapping of operator dynamics and other binding and transport dynamics:

$$k_i(t) = \tilde{\chi}_i(t) O_i(t) \tag{4.8}$$

where $\tilde{\chi}_i(t)$ describes random processes other than that of the operator. For compactness of formalism, I introduce

$$n_i(t) = \frac{k_i(t)}{\gamma_i} = \frac{\tilde{\chi}_i(t)}{\gamma_i} O_i(t) = \chi_i(t) O_i(t) \tag{4.9}$$

Fluctuation of molecular number comes from the third term in eq.(4.7). Z_t is a Brownian motion term that captures the influence of an environment and internal fluctuation. The strength of fluctuation is controlled by $\tilde{\sigma}_i(D_i, t)$. Its explicit form depends on details of the gene network and its environment. It is generally an unknown function before taking any experimental measurement. However, we know that the number of proteins can never go to negative and for large enough system the strength of fluctuation is proportional to square root of the size of the sample, therefore to a reasonable approximation $D_i(t) = \sqrt{D_i}\sigma_i(t)$.

Combining all the above analysis, we obtain a plausible stochastic differential equation for the protein dynamics:

$$dD_i(t) = -\gamma_i(D_i - n_i(t))dt + \sqrt{D_i}\sigma_i(t)dZ_t \tag{4.10}$$

Physically, the equation (4.10) describes a mean reversion process, with a time-dependent mean $n_i(t)$, and it is driven by a Brownian motion with a time-dependent strength.

4.3.2 Operator Dynamics

A second constituent of the model is the dynamics of the operator $O_i(t)$. I describe it as an inhomogenous random telegraph process:

$$\partial_t \begin{bmatrix} P(\alpha_i, t) \\ P(\beta_i, t) \end{bmatrix} = \begin{bmatrix} -\lambda_{i,\beta\alpha} & \lambda_{i,\alpha\beta} \\ \lambda_{i,\beta\alpha} & -\lambda_{i,\alpha\beta} \end{bmatrix} \begin{bmatrix} P(\alpha_i, t) \\ P(\beta_i, t) \end{bmatrix} \tag{4.11}$$

where $P(O_i, t)$ is the probability that the operator is in state O_i and $\lambda_{i,\cdots}$ are functions of D_{i-1} and they can be generally written as

$$\lambda_{i,\alpha\beta} = f_{\alpha\beta}(D_{i-1})\mu_i \tag{4.12a}$$

$$\lambda_{i,\beta\alpha} = f_{\beta\alpha}(D_{i-1})\nu_i \tag{4.12b}$$

where μ_i and ν_i are rate constants.

Consider a positive regulation, where gene i is switched on by binding operator O_i with a protein dimer D_{i-1}:

$$\alpha_i \underset{\nu_i}{\overset{\mu_i}{\rightleftharpoons}} \beta_i + D_{i-1} \tag{4.13}$$

In this case the operator dynamics is

$$\partial_t \begin{bmatrix} P(\alpha_i, t) \\ P(\beta_i, t) \end{bmatrix} = \begin{bmatrix} -\mu_i & \nu_i D_{i-1} \\ \mu_i & -\nu_i D_{i-1} \end{bmatrix} \begin{bmatrix} P(\alpha_i, t) \\ P(\beta_i, t) \end{bmatrix} \tag{4.14}$$

For a negative regulation, where gene i is switched off by binding the operator with D_{i-1}:

$$\alpha_i + D_{i-1} \underset{\nu_i}{\overset{\mu_i}{\rightleftharpoons}} \beta_i \tag{4.15}$$

we have

$$\partial_t \begin{bmatrix} P(\alpha_i, t) \\ P(\beta_i, t) \end{bmatrix} = \begin{bmatrix} -\mu_i D_{i-1} & \nu_i \\ \mu_i D_{i-1} & -\nu_i \end{bmatrix} \begin{bmatrix} P(\alpha_i, t) \\ P(\beta_i, t) \end{bmatrix} \tag{4.16}$$

4.4 Master Equation

The stochastic differential equation for the protein dynamics and random telegraph equation for the operator are formulated from reasonable conjectures. Their validity and applicability cannot be quantified until a fundamental description on the molecular level is presented. The purpose of this section is to treat the one dimensional chain model figure 4-1 in a fundamental way and make connections with the method described in the last section.

4.4.1 Master Equation

We start with defining dynamical variables that specify the gene cascade network. The gene network consists of proteins: X_1, X_2, $\cdots$, X_N, and operators: O_1, O_2, $\cdots$, O_N. There is one additional protein X_0 which is an external control molecule and it regulates the first gene in the network. The state of the system at time t is described by the probability function:

$$P(\vec{n},\vec{O},t) = P(n_1,n_2,\cdots,n_N,O_1,O_2,\cdots,O_N,t;n_0) \tag{4.17}$$

where n_i is the number of protein X_i. For an arbitrary function of n_i: $g(n_i)$, define the creation operator $\mathscr{A}_i$ as

$$\mathscr{A}_i g(n_i) = g(n_i+1) \tag{4.18a}$$

$$\mathscr{A}_i^{-1} g(n_i) = g(n_i-1) \tag{4.18b}$$

We now propose the following assumptions:

Assumption 1 *The number of protein X_i is much larger than the number of operators that it controls so that $n_i \gg 1$.*

Assumption 2 *The transition between two states α and β of an operator occurs on a much faster time scale than the protein processes.*

Assumption 2 allows us to study the protein number fluctuation using a reduced probability function for the proteins only. To achieve that we use conditional probability to rewrite eq.(4.17) as:

$$P(\vec{n},\vec{O},t) = f(\vec{n},t)P(\vec{O},t|\vec{n}) \tag{4.19}$$

Our goal is to find an equation of motion for the reduced probability $f(\vec{n},t)$ of the proteins alone. Let us focus on the i^{th} gene:

$$\alpha_i \xrightarrow{k_i} \alpha_i + X_i \tag{4.20}$$

$$X_i \xrightarrow{\gamma_i} \phi \tag{4.21}$$

$$\alpha_i \underset{\nu_i}{\overset{\mu_i}{\rightleftharpoons}} \beta_i + X_{i-1} \tag{4.22}$$

$$\alpha_{i+1} \underset{\nu_{i+1}}{\overset{\mu_{i+1}}{\rightleftharpoons}} \beta_{i+1} + X_i \tag{4.23}$$

where ϕ represents a sink. Suppressing irrelevant variables, the master equations for (4.20), (4.21) are

$$\partial_t f(n_i,t)P(\alpha_i,t|n_{i-1}) = k_i(\mathscr{A}_i^{-1}-1)f(n_i,t)P(\alpha_i,t|n_{i-1}) + \gamma_i(\mathscr{A}_i-1)n_i f(n_i,t)P(\alpha_i,t|n_{i-1}) \tag{4.24}$$

$$\partial_t f(n_i,t)P(\beta_i,t|n_{i-1}) = \gamma_i(\mathscr{A}_i-1)n_i f(n_i,t)P(\beta_i,t|n_{i-1}) \tag{4.25}$$

Adding (4.24) and (4.25) gives:

$$\partial_t f(n_i,t) = \left[k_i(\mathscr{A}_i^{-1}-1)P(\alpha_i,t|n_{i-1}) + \gamma_i(\mathscr{A}_i-1)n_i\right] f(n_i,t) \tag{4.26}$$

By assumption (1) we can approximate the difference operator as

$$k_i(\mathscr{A}_i^{-1}-1)P(\alpha_i,t|n_{i-1}) \approx k_i P(\alpha_i,t|n_{i-1})(\mathscr{A}_i^{-1}-1) \tag{4.27}$$

to obtain

$$\partial_t f(n_i,t) = \left[k_i P(\alpha_i,t|n_{i-1})(\mathscr{A}_i^{-1}-1) + \gamma_i(\mathscr{A}_i-1)n_i\right] f(n_i,t) \tag{4.28}$$

The reduced probability function $f(n_i,t)$ can be written in a closed form by applying assumption (2), i. e. the transition of an operator between two states is in equilibrium on the time scale of protein dynamics:

$$\Omega^{-1}\nu_i n_{i-1}P(\beta_i,t|n_{i-1}) = \mu_i P(\alpha_i,t|n_{i-1}) \tag{4.29}$$

where Ω is the volume of the system. A second equation comes from the normalization condition:

$$P(\alpha_i,t|n_{i-1}) + P(\beta_i,t|n_{i-1}) = 1 \tag{4.30}$$

We find

$$P(\alpha_i,t|n_{i-1}) = \frac{n_{i-1}}{\Omega\theta_i + n_{i-1}} \tag{4.31}$$

where

$$\theta_i = \frac{\mu_i}{\nu_i} \tag{4.32}$$

Notice that eq.(4.32) takes the form of Hill functions. Combining eq.(4.28) and eq.(4.31) we finally obtain the equation of motion for the reduced probability for proteins $f(\vec{n}, t)$:

$$\partial_t f(\vec{n}, t) = \mathscr{L} f(\vec{n}, t) \tag{4.33}$$

$$\mathscr{L} = \sum_{i=1}^{N} \frac{k_i n_{i-1}}{\Omega\theta_i + n_{i-1}} (\mathscr{A}_i^{-1} - 1) + \gamma_i(\mathscr{A}_i - 1) n_i \tag{4.34}$$

4.4.2 Stochastic Differential Equation

Based on the master equation (4.33) it is desirable to derive a stochastic differential equation for the protein number dynamics and compare it with what we have conjectured in previous sections.

Define $g(c_i, t)$ the probability density function (PDF) of the i^{th} protein's concentration: $c_i = \frac{n_i}{\Omega}$. The following relation is clear:

$$g(c_i, t) dc_i = g(c_i, t) \frac{1}{\Omega} = f(n_i, t) \tag{4.35}$$

as the concentration can only change by multiples of $\frac{1}{\Omega}$. In other words, we have

$$dc_i \sim \frac{1}{\Omega} \tag{4.36}$$

The creation operator $\mathscr{A}_i$ in the this continuum limit has the form:

$$\mathscr{A}_i \to \exp\left(\Omega^{-1}\partial_{c_i}\right) \tag{4.37}$$

This correspondence is clearly shown as the following, for an arbitrary function $u(n_i)$:

$$\begin{aligned}\mathscr{A}_i u(n_i) &= u(n_i+1) \\ &= \sum_{k=0}^{\infty} \frac{1}{k!} \partial_{n_i}^{k} u(n_i) \\ &= \sum_{k=0}^{\infty} \frac{\Omega^{-k}}{k!} \partial_{c_i}^{k} u(n_i) \\ &= \exp\left(\Omega^{-1}\partial_{c_i}\right) u(n_i) \end{aligned} \tag{4.38}$$

Using (4.35) and (4.37) to (4.33) and (4.34) we find by expanding the series:

$$\begin{aligned}\Omega^{-1}\partial_t g(c_i,t) &= \frac{k_i c_{i-1}}{\theta_i + c_{i-1}} \left(-\Omega^{-1}\partial_{c_i} + \frac{1}{2}\Omega^{-2}\partial_{c_i}^{2}\right) \Omega^{-1} g(c_i,t) \\ &+ \gamma_i \left(\Omega^{-1}\partial_{c_i} + \frac{1}{2}\Omega^{-2}\partial_{c_i}^{2}\right) c_i g(c_i,t) + \cdots \end{aligned} \tag{4.39}$$

For sufficiently large volume of a system we can truncate the series to 2^{nd} order to obtain:

$$\begin{aligned}\partial_t g(c_i,t) = &- \partial_{c_i}\left[\left(\frac{k_i c_{i-1}\Omega^{-1}}{\theta_i + c_{i-1}} - \gamma_i c_i\right) g(c_i,t)\right] \\ &+ \frac{1}{2}\partial_{c_i}^{2}\left[\left(\frac{k_i c_{i-1}\Omega^{-2}}{\theta_i + c_{i-1}} + \Omega^{-1}\gamma_i c_i\right) g(c_i,t)\right] \end{aligned} \tag{4.40}$$

Equation (4.40) takes the form of Fokker-Planck equation and it can be converted to a stochastic differential equation:

$$dc_i(t) = -\gamma_i \left(c_i(t) - \frac{\gamma_i^{-1}\Omega^{-1}k_i c_{i-1}(t)}{\theta_i + c_{i-1}(t)}\right) dt + \sqrt{\frac{\Omega^{-2}k_i c_{i-1}(t)}{\theta_i + c_{i-1}(t)} + \Omega^{-1}\gamma_i c_i(t)}\; dZ_{i,t} \tag{4.41}$$

or equivalently

$$dn_i(t) = -\gamma_i \left(n_i(t) - \frac{\gamma_i^{-1}k_i n_{i-1}(t)}{\Omega\theta_i + n_{i-1}(t)}\right) dt + \sqrt{\frac{k_i n_{i-1}(t)}{\Omega\theta_i + n_{i-1}(t)} + \gamma_i n_i(t)}\; dZ_{i,t} \tag{4.42}$$

Comparing (4.42) with (4.10), we find our conjecture for the form of stochastic differential equation is correct for large values of $n_i(t)$. For small values of $n_i(t)$, the applicability of stochastic differential equation is dubious and one should use the master equation instead.

4.5 Ω-Expansion

The master equation is generally difficult to solve and one way to solve it is to use the Ω-expansion, where Ω is the volume of the system. As can be expected, fluctuations depend on the size of the system, therefore a Ω-expansion relies on the smallness of fluctuations.

4.5.1 Derivation

The standard Ω-expansion starts from the following time-dependent transformation:

$$\vec{n} = \Omega\vec{\phi}(t) + \Omega^{\frac{1}{2}}\vec{\xi} \tag{4.43}$$

where $\vec{\phi}(t) = (\phi_1(t), \phi_2(t), \cdots, \phi_N(t))$ is a deterministic part which corresponds to a macroscopic variable. $\vec{\xi} = (\xi_1, \xi_2, \cdots, \xi_N)$ is a fluctuation part, which becomes less important as Ω increases. In terms of new variables, the reduced probability $f(\vec{n}, t)$ transforms to

$$f(\vec{n}, t) = f\left(\Omega\vec{\phi}(t) + \Omega^{\frac{1}{2}}\vec{\xi}, t\right) = \rho(\vec{\xi}, t) \tag{4.44}$$

The creation operator $\mathscr{A}_i$ which maps $n_i \to n_i + 1$ corresponds to mapping $\xi_i \to \xi_i + \Omega^{-\frac{1}{2}}$ and has the following representation:

$$\mathscr{A}_i = \exp\left[\Omega^{-\frac{1}{2}}\partial_{\xi_i}\right] \tag{4.45a}$$

$$\mathscr{A}_i^{-1} = \exp\left[-\Omega^{-\frac{1}{2}}\partial_{\xi_i}\right] \tag{4.45b}$$

Also the transformation of the time derivative takes the form:

$$\partial_t f(\vec{n}, t) = \partial_t \rho(\vec{\xi}, t) - \Omega^{\frac{1}{2}} \sum_{i=1}^{N} \dot{\phi}_i \partial_{\xi_i} \rho(\vec{\xi}, t) \tag{4.46}$$

It is worth noticing that the 2^{nd} term in (4.46) arises because $\partial_t f(\vec{n}, t)$ takes partial derivative with respect to t while holding $\vec{n}$ fixed. Therefore the contribution from $\vec{\phi}(t)$ should be subtracted.

In new variables, the master equation becomes

$$\partial_t \rho(\vec{\xi}, t) = \mathscr{D}\rho(\vec{\xi}, t) \tag{4.47}$$

where the differential operator $\mathscr{D}$ is

$$\begin{aligned} \mathscr{D} \; = \; & \Omega^{\frac{1}{2}} \sum_{i=1}^{N} \dot{\phi}_i \partial_{\xi_i} + \sum_{i=2}^{N} \frac{k_i(\phi_{i-1} + \Omega^{-\frac{1}{2}}\xi_{i-1})}{\theta_i + \phi_{i-1} + \Omega^{-\frac{1}{2}}\xi_{i-1}} \left[\exp\left(-\Omega^{-\frac{1}{2}}\partial_{\xi_i}\right) - 1\right] \\ & + \frac{k_1\phi_0}{\theta_1 + \phi_0} \left[\exp\left(-\Omega^{-\frac{1}{2}}\partial_{\xi_i}\right) - 1\right] + \sum_{i=1}^{N} \gamma_i \left[\exp\left(\Omega^{-\frac{1}{2}}\partial_{\xi_i}\right) - 1\right] (\Omega\phi_i + \Omega^{\frac{1}{2}}\xi_i) \end{aligned} \tag{4.48}$$

Before we can correctly expand $\mathscr{D}$ in power series of Ω^{-1}, special care must be taken about k_i, which is defined as the rate per volume. We must identify its order in terms of Ω. Recall that in our model there is only one copy of each gene. The rate of protein synthesis is

$$\Omega k_i \cdot \frac{1}{\Omega} = k_i$$

while the rate of protein degradation is

$$\Omega\gamma_i \cdot \frac{n_i}{\Omega} = \gamma_i n_i$$

In steady state these two rates equal: $k_i = \gamma_i \langle\phi_i\rangle_s \Omega$, so

$$\frac{k_i}{\gamma_i} \sim \mathcal{O}(\Omega) \tag{4.49}$$

Thus we define the following rate constant:

$$\kappa_i = \frac{k_i}{\Omega} \tag{4.50}$$

which is on the same order as γ_i. Then the differential operator $\mathscr{D}$ becomes:

$$\begin{aligned}\mathscr{D} \;=\; & \Omega^{\frac{1}{2}} \sum_{i=1}^{N} \dot{\phi}_i \partial_{\xi_i} + \sum_{i=2}^{N} \frac{\Omega \kappa_i (\phi_{i-1} + \Omega^{-\frac{1}{2}} \xi_{i-1})}{\theta_i + \phi_{i-1} + \Omega^{-\frac{1}{2}} \xi_{i-1}} \left[\exp\left(-\Omega^{-\frac{1}{2}} \partial_{\xi_i}\right) - 1\right] \\ & + \frac{\Omega \kappa_1 \phi_0}{\theta_1 + \phi_0} \left[\exp\left(-\Omega^{-\frac{1}{2}} \partial_{\xi_i}\right) - 1\right] + \sum_{i=1}^{N} \gamma_i \left[\exp\left(\Omega^{-\frac{1}{2}} \partial_{\xi_i}\right) - 1\right] (\Omega \phi_i + \Omega^{\frac{1}{2}} \xi_i)\end{aligned} \tag{4.51}$$

Now expand $\mathscr{D}$ in powers of Ω:

$$\frac{\Omega \kappa_i \phi_{i-1}}{\theta_i + \phi_{i-1} + \Omega^{-1/2} \xi_{i-1}} = \kappa_i \phi_{i-1} \sum_{n=1}^{\infty} (-1)^{n-1} \frac{\Omega^{\frac{3-n}{2}} \xi_{i-1}^{n-1}}{(\theta_i + \phi_{i-1})^n}$$

$$\frac{\Omega^{\frac{1}{2}} \kappa_i \phi_{i-1}}{\theta_i + \phi_{i-1} + \Omega^{-1/2} \xi_{i-1}} = \kappa_i \sum_{n=1}^{\infty} (-1)^{n-1} \frac{\Omega^{1-\frac{n}{2}} \xi_{i-1}^{n-1}}{(\theta_i + \phi_{i-1})^n}$$

$$\exp\left(\pm \Omega^{-\frac{1}{2}} \partial_{\xi_i}\right) - 1 = \sum_{n=1}^{\infty} \frac{(\pm 1)^n}{n!} \Omega^{-\frac{n}{2}} \partial_{\xi_i}^n$$

$$\frac{\Omega \kappa_1 \phi_0}{\theta_1 + \phi_0} \left[\exp\left(\Omega^{-\frac{1}{2}} \partial_{\xi_1}\right) - 1\right] = \frac{\kappa_1 \phi_0}{\theta_1 + \phi_0} \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \Omega^{1-\frac{n}{2}} \partial_{\xi_1}^n$$

$$\Omega \gamma_i \left[\exp\left(\Omega^{-\frac{1}{2}} \partial_{\xi_1}\right) - 1\right] (\phi_i + \Omega^{-\frac{1}{2}} \xi_i) = \gamma_i \left(\sum_{n=1}^{\infty} \frac{\phi_i \Omega^{1-\frac{n}{2}}}{n!} \partial_{\xi_i}^n + \sum_{n=1}^{\infty} \frac{\xi_i \Omega^{\frac{1-n}{2}}}{n!} \partial_{\xi_i}^n \right)$$

Collecting terms in powers of Ω:

$\boxed{\Omega^{\frac{1}{2}}}$

$$\left[\sum_{i=1}^{N} \dot{\phi}_i \partial_{\xi_i} - \sum_{i=2}^{N} \frac{\kappa_i \phi_{i-1}}{\theta_i + \phi_{i-1}} \partial_{\xi_i} - \frac{\kappa_1 \phi_0}{\theta_1 + \phi_0} \partial_{\xi_1} + \sum_{i=1}^{N} \gamma_i \partial_{\xi_i} \right] \rho(\vec{\xi}, t) = 0$$

This equation is satisfied identically if

$$\dot{\phi}_i = \frac{\kappa_i \phi_{i-1}}{\theta_i + \phi_{i-1}} - \gamma_i \phi_i \qquad i = 1, \cdots, N \tag{4.52}$$

Equation (4.52) is just the macroscopic law of gene cascade kinetics.

$\boxed{\Omega^0}$

$$\begin{aligned} \partial_t \rho(\vec{\xi}, t) = & - \sum_{i=1}^{N} \partial_{\xi_i} \left[\frac{\kappa_i \xi_{i-1}}{\theta_i + \phi_{i-1}} - \frac{\kappa_i \phi_{i-1} \xi_{i-1}}{(\theta_i + \phi_{i-1})^2} - \gamma_i \xi_i \right] \rho(\vec{\xi}, t) \\ & + \frac{1}{2} \sum_{i=1}^{N} \partial^2_{\xi_i} \left[\frac{\kappa_i \phi_{i-1}}{\theta_i + \phi_{i-1}} + \gamma_i \phi_i \right] \rho(\vec{\xi}, t) \end{aligned} \tag{4.53}$$

Since $\rho(\vec{\xi}, t)$ has the interpretation of the probability distribution of fluctuation $\vec{\xi}$, (4.53) is the Fokker-Planck equation. Notice the external fluctuation affects the gene cascade through $\xi_0(t)$ and its dynamics is often known.

We now quantitatively discuss the statistics of fluctuation in and out of equilibrium. Multiply ξ_i to both sides of eq.(4.53) and integrate $\vec{\xi}$ (by parts) to find:

$$\partial_t \langle \xi i(t) \rangle = \frac{\kappa_i}{\theta_i + \phi_{i-1}} \left(1 - \frac{\phi_{i-1}}{\theta_i + \phi_{i-1}} \right) \langle \xi_{i-1}(t) \rangle - \gamma_i \langle \xi i(t) \rangle \tag{4.54}$$

It is clearly seen that two sources contribute to the the dynamics of fluctuation at site i: upstream fluctuation which is transmitted through gene $i-1$ and a decay of fluctuation at site i, made possible by the degradation reaction.

The correlation function of fluctuations at two sites can be calculated by multiplying $\xi_i \xi_j$ to both sides of eq.(4.53) and integrate $\vec{\xi}$, we find

$$\begin{aligned} \partial_t \langle \xi_i(t) \xi_j(t) \rangle = & - (\gamma_i + \gamma_j) \langle \xi_i(t) \xi_j(t) \rangle + \frac{\kappa_i}{\theta_i + \phi_{i-1}} \left(1 - \frac{\phi_{i-1}}{\theta_i + \phi_{i-1}} \right) \langle \xi_{i-1}(t) \xi_j(t) \rangle \\ & + \frac{\kappa_j}{\theta_j + \phi_{j-1}} \left(1 - \frac{\phi_{j-1}}{\theta_j + \phi_{j-1}} \right) \langle \xi_i(t) \xi_{j-1}(t) \rangle + \delta_{ij} \left(\frac{\kappa_i \phi_{i-1}}{\theta_i + \phi_{i-1}} + \gamma_i \phi_i \right) \end{aligned} \tag{4.55}$$

To study the structure and solution to equation (4.55), I define the $H-$matrix:

$$H = -\Gamma + T(t) \tag{4.56}$$

The decay matrix Γ has matrix element:

$$\Gamma_{ij} = \gamma_i \delta_{ij} \tag{4.57}$$

and the transition matrix $T-$matrix is defined as

$$T_{ij}(t) = \frac{\kappa_i}{\theta_i + \phi_j(t)} \left[1 - \frac{\phi_j(t)}{\theta_i + \phi_j(t)} \right] \delta_{i-1,j} \tag{4.58}$$

Define the $Q-$matrix as

$$Q_{ij}(t) = \left[\frac{\kappa_i \phi_{i-1}(t)}{\theta_i + \phi_{i-1}(t)} + \gamma_i \phi_i(t) \right] \delta_{ij} \tag{4.59}$$

Then the fluctuation matrix M defined as

$$M_{ij} = \langle \xi_i(t) \xi_j(t) \rangle \tag{4.60}$$

satisfies

$$\frac{dM(t)}{dt} = H(t)M(t) + M(t)H^T(t) + Q(t) = \mathscr{L}_H(t)M(t) + Q(t) \tag{4.61}$$

where a superscript T denotes transpose. $\mathscr{L}_H$ is the fluctuation superoperator defined as

$$\mathscr{L}_H(t)M(t) = H(t)M(t) + M(t)H^T(t) \tag{4.62}$$

The fluctuation superoperator can be explicitly defined as the following:

$$\left(\mathscr{L}_H(t)M(t)\right)_{mn} = \sum_{i,j} \mathscr{L}_H(t)_{mn,ij} M(t)_{ij} \tag{4.63a}$$

$$\mathscr{L}_H(t)_{mn,ij} = H_{mi}\delta_{jn} + \delta_{mi}H_{jn}^T \tag{4.63b}$$

The fluctuation matrix can be formally solved to be:

$$M(t) = \mathcal{T}_\tau \exp\left(\int_0^t d\tau \mathscr{L}_H(\tau)\right) M(0) + \int_0^t d\tau \mathcal{T}_s \exp\left(\int_\tau^t ds \mathscr{L}_H(s)\right) Q(\tau) \tag{4.64}$$

where $\mathcal{T}_\tau$ is the usual time ordering operator defined in quantum mechanics and field theory.

To theoretically analyze the formal solution of $M(t)$ in eq.(4.64) it is convenient to introduce two super operators:

$$\mathscr{L}_\Gamma M(t) = \Gamma M(t) + M(t)\Gamma \tag{4.65}$$

$$\mathscr{L}_T(t)M(t) = T(t)M(t) + M(t)T^T(t) \tag{4.66}$$

Decompose the fluctuation matrix into a diagonal part $M^{(d)}(t)$, describing the variance of fluctuation at each site of the cascade, and an off diagonal part $M^{(od)}(t)$ which describes covariant fluctuations between two sites:

$$M(t) = M^{(d)}(t) + M^{(od)}(t) \tag{4.67}$$

This decomposition can be achieved by the method of projection operator defined by

$$\mathcal{P} = \delta_{mn}\delta_{mi}\delta_{nj} \tag{4.68}$$

such that

$$M^{(d)}(t) = \mathcal{P}M(t) \tag{4.69a}$$

$$M^{(od)}(t) = (1 - \mathcal{P})M(t) \tag{4.69b}$$

Multiplying (4.61) by $\mathcal{P}$ gives

$$\begin{aligned}\frac{dM^{(d)}(t)}{dt} &= \mathcal{P}\mathscr{L}_H(t)\mathcal{P}M(t) + \mathcal{P}\mathscr{L}_H(t)(1-\mathcal{P})M(t) + \mathcal{P}Q(t)\\ &= \mathcal{P}\mathscr{L}_H(t)M^{(d)}(t) + \mathcal{P}\mathscr{L}_H(t)M^{(od)}(t) + \mathcal{P}Q(t) \end{aligned} \tag{4.70}$$

Multiply (4.61) by $1-\mathcal{P}$:

$$\frac{dM^{(od)}(t)}{dt} = (1-\mathcal{P})\mathscr{L}_H(t)M^{(d)}(t) + (1-\mathcal{P})\mathscr{L}_H(t)M^{(od)}(t) + (1-\mathcal{P})Q(t)$$

Since $Q(t)$ is diagonal, $(1-\mathcal{P})Q(t) = 0$ and $\mathcal{P}Q(t) = Q(t)$, therefore

$$\frac{dM^{(od)}(t)}{dt} = (1-\mathcal{P})\mathscr{L}_H(t)M^{(d)}(t) + (1-\mathcal{P})\mathscr{L}_H(t)M^{(od)}(t) \tag{4.71}$$

The equation (4.71) has a formal solution

$$\begin{aligned}M^{(od)}(t) &= \int_0^t dt_1 \mathcal{T}_{t_2} \exp\left[\int_{t_1}^t dt_2 (1-\mathcal{P})\mathscr{L}_H(t_2)\right](1-\mathcal{P})\mathscr{L}_H(t_1)M^{(d)}(t_1)\\ &\quad + \mathcal{T}_{t_1}\exp\left[\int_0^t dt_1(1-\mathcal{P})\mathscr{L}_H(t_1)\right]M^{(od)}(0) \end{aligned} \tag{4.72}$$

Suppose that genes are not correlated to each other at time 0 but are under their own internal fluctuations then $M^{(od)}(0) = 0$. The 2^{nd} term in (4.72) vanishes. Substituting (4.72) into (4.70), we get

$$\begin{aligned}\frac{dM^{(d)}(t)}{dt} &= \mathcal{P}\mathscr{L}_H(t)\int_0^t dt_1 \mathcal{T}_{t_2}\exp\left[\int_{t_1}^t dt_2(1-\mathcal{P})\mathscr{L}_H(t_2)\right](1-\mathcal{P})\mathscr{L}_H(t_1)M^{(d)}(t_1)\\ &\quad + \mathcal{P}\mathscr{L}_H M^{(d)}(t) + Q(t)\end{aligned}$$

Notice we have the following relations:

$$\mathcal{P}\mathscr{L}_T M^{(d)} = 0$$

$$\mathcal{P}\mathscr{L}_\Gamma M^{(d)} = \mathscr{L}_\Gamma M^{(d)}$$

$$(1-\mathcal{P})\mathscr{L}_\Gamma M^{(d)} = 0$$

$$(1-\mathcal{P})\mathscr{L}_T M^{(d)} = \mathscr{L}_T M^{(d)}$$

$$\mathcal{P}\mathscr{L}_H(1-\mathcal{P}) = \mathcal{P}\mathscr{L}_T(1-\mathcal{P})$$

We obtain a closed differential equation for $M^{(d)}(t)$:

$$\begin{aligned} \frac{dM^{(d)}(t)}{dt} &= -\mathscr{L}_\Gamma M^{(d)}(t) + Q(t) \\ &\quad + \mathscr{L}_T(t) \int_0^t dt_1 \mathcal{T}_{t_2} \exp\left[\int_{t_1}^t dt_2 (1-\mathcal{P})\mathscr{L}_H(t_2)\right] \mathscr{L}_T(t_1) M^{(d)}(t_1) \end{aligned} \tag{4.74}$$

Equation (4.74) shows non-Markovian nature of the diagonal fluctuation matrix. The sources of fluctuation come from internal noise at each site and transmitted upstream fluctuation. It is worth pointing out that transmissions of the fluctuations is realized only through off-diagonal coupling.

When the macroscopic quantities such as $\phi_i(t)$ are in steady state, $\mathscr{L}_H$ and Q are independent of time. However, the fluctuation $M(t)$ can still evolve in time:

$$\begin{aligned} \frac{dM^{(d)}(t)}{dt} &= -\mathscr{L}_\Gamma M^{(d)}(t) + Q \\ &\quad + \mathscr{L}_T \int_0^t dt_1 \exp\left[(1-\mathcal{P})\mathscr{L}_H \cdot (t-t_1)\right] \mathscr{L}_T M^{(d)}(t_1) \end{aligned} \tag{4.75}$$

One way to solve (4.75) is by method of Laplace transformation:

$$\widehat{M}^{(d)}(s) = \int_0^\infty dt\, e^{-st} M^{(d)}(t) \tag{4.76}$$

then (4.75) becomes

$$s\widehat{M}^{(d)}(s) - M^{(d)}(0) = -\mathscr{L}_\Gamma \widehat{M}^{(d)}(s) + \frac{Q}{s} + \mathscr{L}_T \frac{1}{s-(1-\mathcal{P})\mathscr{L}_H} \mathscr{L}_T \widehat{M}^{(d)}(s) \tag{4.77}$$

so

$$\widehat{M}^{(d)}(s) = \frac{1}{s + \mathscr{L}_\Gamma - \mathscr{L}_T \frac{1}{s-(1-\mathcal{P}).\mathscr{L}_H} \mathscr{L}_T} \left[\frac{Q}{s} + M^{(d)}(0) \right] \tag{4.78}$$

$M^{(d)}(t)$ is obtained from inverse Laplace transformation of (4.78). Let us examine the case when $M^{(d)}(t)$ reaches steady state, i. e. $M_{st}^{(d)} = M^{(d)}(\infty)$. Using the fact for any $f(t)$:

$$s\hat{f}(s) = \int_0^\infty dx\ e^{-x} f(\frac{x}{s})$$

$$\lim_{s\longrightarrow 0} s\hat{f}(s) = \lim_{s\longrightarrow 0} \int_0^\infty dx\ e^{-x} f(\frac{x}{s}) = f(\infty) \int_0^\infty dx\ e^{-x} = f(\infty)$$

we find

$$M_{st}^{(d)} = \frac{1}{\mathscr{L}_\Gamma + \mathscr{L}_T \frac{1}{(1-\mathcal{P})(\mathscr{L}_T - \mathscr{L}_\Gamma)} \mathscr{L}_T} Q \tag{4.80}$$

(4.80) being formal and exact, it is still hard to analyze the underlying process, therefore we seek approximations to (4.74).

4.5.2 Markovian Approximation

The difficulty in (4.74) and (4.75)arises from the non-markovian nature of the fluctuation matrix. To motive the Markovian approximation consider the following integral:

$$I = \int_0^t dt_1 e^{-\alpha(t-t_1)} f(t_1), \qquad \alpha \gg 1 \tag{4.81}$$

The weight function (memory kernel) is exponential which kills the contribution of $f(t_1)$ at small t_1 to the integral. In the large α limit:

$$\begin{aligned} I &= \int_0^t dt_1 e^{-\alpha t_1} f(t - t_1) \\ &= \frac{1}{\alpha} \int_0^{\alpha t} dx e^{-x} f(t - \frac{x}{\alpha}) \\ &\approx \frac{1}{\alpha} \int_0^\infty dx e^{-x} f(t) \\ &= \frac{1}{\alpha} f(t) \end{aligned} \tag{4.82}$$

This is the Markovian approximation we would like to apply to (4.74) and (4.75).

If the matrix element of $T-$matrix is much smaller than that of $\Gamma-$matrix:

$$\frac{\kappa_i}{\theta_i + \phi_{i-1}}\left(1 - \frac{\phi_{i-1}}{\theta_i + \phi_{i-1}}\right) \ll \gamma_i \tag{4.83}$$

which means each gene synthesizes quite a large number of proteins and the influence of upstream fluctuation is much smaller than the internal fluctuation at each gene. This is possible in a reasonably large system. To quantify this condition notice that in steady state of ϕ_i:

$$\frac{\kappa_i \phi_{i-1}}{\theta_i + \phi_{i-1}} = \gamma_i \phi_i \tag{4.84}$$

Substituting this to (4.83) gives

$$\frac{\phi_i}{\phi_{i-1}}\left(1 - \frac{\phi_{i-1}}{\theta_i + \phi_{i-1}}\right) \ll 1 \Longleftrightarrow \phi_{i-1} \gg \theta_i \tag{4.85}$$

Recall $\theta_i = \mu_i/\nu_i$, so in order to apply Markovian approximation we must require

$$\phi_{i-1}\nu_i \gg \mu_i \tag{4.86}$$

That is the operator of gene i exists in the on-state most of the time.

Under the Markovian approximation (4.74) becomes

$$\frac{dM^{(d)}(t)}{dt} = -\mathscr{L}_\Gamma M^{(d)}(t) + Q(t) + \mathscr{L}_T(t)\frac{1}{(1-\mathcal{P})\mathscr{L}_H(t)}\mathscr{L}_T(t)M^{(d)}(t) \tag{4.87}$$

Given $\| \mathscr{L}_\Gamma \| \gg \| \mathscr{L}_T \|$, we have

$$\frac{1}{(1-\mathcal{P})(\mathscr{L}_\Gamma + \mathscr{L}_T)} = \frac{1}{1 + \mathscr{L}_\Gamma^{-1}\mathscr{L}_T}\frac{1}{(1-\mathcal{P})\mathscr{L}_\Gamma} \tag{4.88}$$

Since it is the off-diagonal subspace to which $[(1-\mathcal{P})\mathscr{L}_\Gamma]^{-1}$ acts is nonvanishing and $\mathscr{L}_T M^{(d)}$

is already in that space it follows that

$$\begin{aligned}
& \mathscr{L}_T(t)\left[(1-\mathcal{P})(\mathscr{L}_\Gamma+\mathscr{L}_T)\right]^{-1}\mathscr{L}_T(t)M^{(d)}(t) \\
= & \mathscr{L}_T(t)\left(1+\mathscr{L}_\Gamma^{-1}\mathscr{L}_T\right)^{-1}\mathscr{L}_\Gamma^{-1}\mathscr{L}_T(t)M^{(d)}(t) \\
= & \sum_{n=1}^{\infty}(-1)^n\mathscr{L}_T(t)\left[\mathscr{L}_\Gamma^{-1}\mathscr{L}_T(t)\right]^n\mathscr{L}_\Gamma^{-1}\mathscr{L}_T(t)M^{(d)}(t)
\end{aligned} \tag{4.89}$$

To lowest order in $\mathscr{L}_\Gamma^{-1}\mathscr{L}_T(t)$:

$$\frac{dM^{(d)}(t)}{dt} = -\mathscr{L}_\Gamma M^{(d)}(t) + Q(t) + \mathscr{L}_T(t)\mathscr{L}_\Gamma^{-1}\mathscr{L}_T(t)M^{(d)}(t) \tag{4.90}$$

where

$$\left(\mathscr{L}_\Gamma^{-1}\right)_{ij,mn} = \frac{1}{\gamma_i+\gamma_j}\delta_{im}\delta_{jn} \tag{4.91}$$

(4.90) is our Markovian approximation result.

4.5.3 Fluctuation Transmission and Bound

In this section we will study the transmission property of gene cascade within our Markovian approximation. In the steady state, we obtain a recursion relation from (4.90):

$$M_{st}^{(d)} = \mathscr{L}_\Gamma^{-1}Q + \mathscr{L}_\Gamma^{-1}\mathscr{L}_T\mathscr{L}_\Gamma^{-1}\mathscr{L}_T M_{st}^{(d)} \tag{4.92}$$

or explicitly:

$$M_{kk} = a_k + b_k M_{k-1\ k-1} \tag{4.93}$$

with

$$a_k = \frac{Q_{kk}}{2\gamma_k} \tag{4.94a}$$

$$b_k = \frac{1}{\gamma_k(\gamma_k+\gamma_{k-1})}T_{k\ k-1}^2 \tag{4.94b}$$

a_k is the amplitude of fluctuation generated by gene expression at site k alone, while b_k is the transmission efficiency from gene $k-1$ to k.

By iteration, we find

$$M_{nn} = \sum_{i=1}^{n} \left(a_i \prod_{j=i+1}^{n} b_j \right) \tag{4.95}$$

Equation (4.95) has the following interpretation: The fluctuation at gene n is a sum of all upstream fluctuations weighted by the product of transmission coefficient of each gene in between.

Equation (4.95) also predicts an upper bound for the fluctuation in this gene cascade network. Denote $\bar{a} = \sup a_i$ and $\bar{b} = \sup b_i$ then

$$M_{NN} \leq \bar{a} \sum_{i=1}^{N} \bar{b}^{i-1} = \frac{\bar{a}(1-\bar{b}^N)}{1-\bar{b}} \tag{4.96}$$

In the limit $N \to \infty$:

$$M_\infty \leq \frac{\bar{a}}{1-\bar{b}} \tag{4.97}$$

4.6 Discussion

In this work, I study the fluctuation of protein numbers in a gene cascade. There are two types of fluctuation: one originates from the coupling with external sources and the second one is almost independent of environments and the fluctuation exists even when there is no coupling with external source. The second type is caused by random collisions between molecules that initiates the chemical and biological reactions. This type of fluctuation can not be simply removed by reducing the coupling with external worlds and therefore is intrinsic. In the following, when we refer to fluctuation we mean the second type of fluctuation. The fluctuation is increasingly important when the volume of the system is sufficiently small and there are only tens of molecules. Figure 4-3 shows a simulation of the fluctuation of protein numbers (monomer and dimer) synthesized by a single gene, which in turn is self-regulated by the protein (dimer). There is no coupling to an external source and the time trajectory clearly shows the intrinsic fluctuation. When genes are coupled the analysis of fluctuation become more difficult. I show in the work that several approaches can be used:

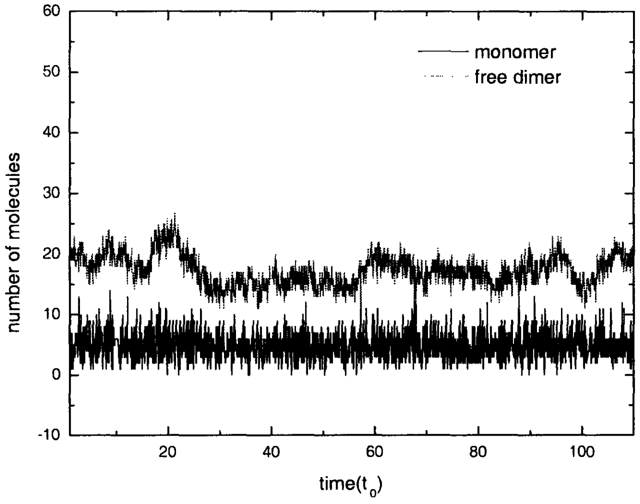

Figure 4-3: Time Trajectories of Protein Numbers by Simulation

stochastic differential equation and master equation. The construction of the stochastic differentia equations is mostly built on intuition and it has the advantage of numerical feasibility. The master equation approach is more fundamental but it is very hard to implement numerically. Nevertheless if the size of the system is not too small, certain approximations can be applied. In this work, I use the $\Omega-$expansion to study the fluctuation propagation through a gene cascade network. As can be seen from (4.53), which is a Fokker-Planck equation, the $\Omega-$expansion is essentially a gaussian noise approximation around a solution of macroscopic variables. The validity of this expansion is up to experimental and numerical tests. In figure 4-4 I plot the distribution of protein dimers from the simulation of a single self-regulatory gene network. Also a gaussian fit is given in this figure. It is clear that gaussian noise approximation is a good approximation to protein dimer number which is on the order of 18 molecules. When the number of a protein molecules goes down, the deviation from gaussian is expected to be prominent. Figure 4-5 shows the distribution of protein monomer number obtained from computer simulation. It is found that when on

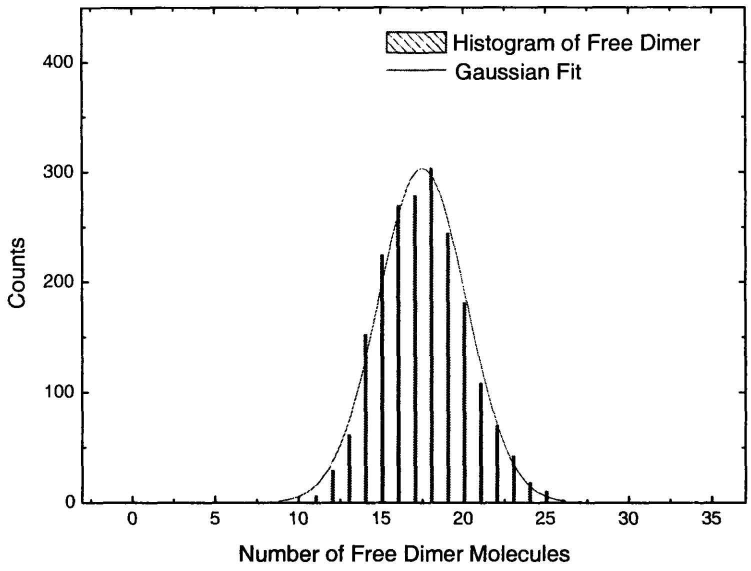

Figure 4-4: Protein Dimer Number Distribution and Gaussian Fit. The histogram is obtained from computer simulation and a gaussian distribution fits well to the histogram.

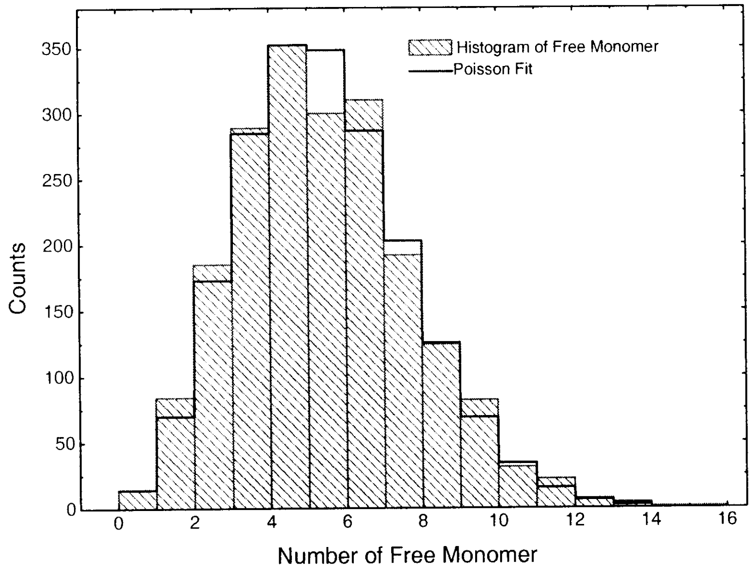

Figure 4-5: Protein Monomer Number Distribution and Poisson Fit. The histogram is obtained from computer simulation. A gaussian distribution cannot fit the histogram. A good fit can be obtained by a Poisson distribution.

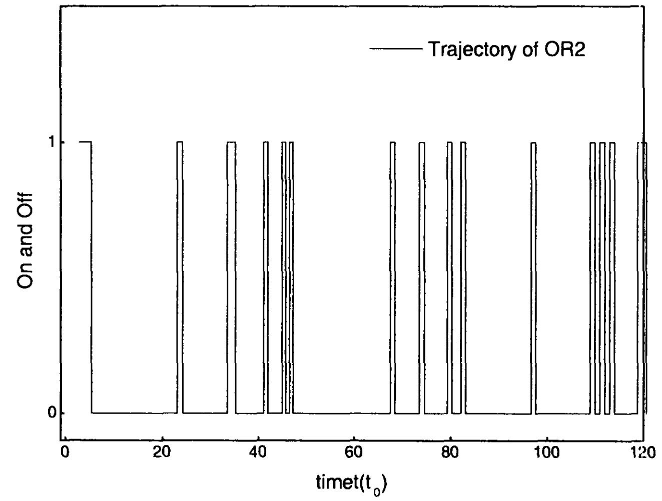

Figure 4-6: The trajectory of the active operator state O_{R_2} shows an on and off dynamics. See appendix for detailed description.

average only 6 molecules are synthesized the statistics of fluctuation can not be described by gaussian and instead a poisson distribution is needed. In a typical gene network the number of protein molecules is on the order 50, therefore the $\Omega-$expansion is a reasonable method to study these systems. The trajectory of the operator dynamics is shown in figure 4-6.

Based on the $\Omega-$expansion, I further look at the Markovian approximation to the equation of motion of the diagonal fluctuation matrix $M^{(d)}$. This approximation is valid when the coupling of genes is weak enough so that the dominant fluctuation of at each gene site is its intrinsic fluctuation. In this case, I find an upper bound for the end chain fluctuation and this result is in agreement with the results from the stochastic differential equation approach. [8] In this case, a transmission coefficient can be defined for each gene which controls the fluctuation conductance.

4.7 Appendix: Simulation of Self-regulatory Gene Network

In this appendix, I will discuss in detail the simulation that is used in the main part of this chapter for a regulatory gene network. The regulatory gene network consists of a single gene. The gene can be expressed to synthesize protein monomer $\mathcal{M}$ and the monomer can consequently react to form dimer $\mathcal{D}$ or simply degrade. The basic reactions are the following:

$$\mathcal{M} + \mathcal{M} \underset{\theta_1 k_1}{\overset{k_1}{\rightleftharpoons}} \mathcal{D} \tag{4.98}$$

$$\mathcal{O}_{R_0} + \mathcal{D} \underset{\theta_2 k_2}{\overset{k_2}{\rightleftharpoons}} \mathcal{O}_{R_1} \tag{4.99}$$

$$\mathcal{O}_{R_1} + \mathcal{D} \underset{\theta_3 k_3}{\overset{k_3}{\rightleftharpoons}} \mathcal{O}_{R_2} \tag{4.100}$$

$$\mathcal{O}_{R_2} + \mathcal{D} \underset{\theta_4 k_4}{\overset{k_4}{\rightleftharpoons}} \mathcal{O}_{R_3} \tag{4.101}$$

$$\mathcal{M} \xrightarrow{k_5} \phi \tag{4.102}$$

$$\mathcal{O}_{R_1} \xrightarrow{k_6} \mathcal{O}_{R_1} + \mathcal{M} \tag{4.103}$$

$$\mathcal{O}_{R_2} \xrightarrow{k_7} \mathcal{O}_{R_2} + \mathcal{M} \tag{4.104}$$

The operator $\mathcal{O}$ can exist in four states $\{\mathcal{O}_{R_0}, \mathcal{O}_{R_1}, \mathcal{O}_{R_2}, \mathcal{O}_{R_3}\}$. $\mathcal{O}_{R_0}$ is an off state where no protein monomer $\mathcal{M}$ can be synthesized. When $\mathcal{O}_{R_0}$ binds with a protein dimer $\mathcal{D}$ it becomes $\mathcal{O}_{R_1}$ and protein monomer $\mathcal{M}$ can be synthesized only on a base level. When more protein dimers are available $\mathcal{O}_{R_1}$ can bind with the dimers to form $\mathcal{O}_{R_2}$ and in this state protein monomer can be massively synthesized. However, when the number of protein dimers reaches a certain upper bound, $\mathcal{O}_{R_2}$ will bind with the excessive dimer to form $\mathcal{O}_{R_3}$ and in this state no protein monomer can be synthesized. Therefore $\mathcal{O}_{R_3}$ is also an off state. The

Reaction	$\mathcal{M}$	$\mathcal{D}$	$\mathcal{O}_{R_0}$	$\mathcal{O}_{R_1}$	$\mathcal{O}_{R_2}$	$\mathcal{O}_{R_3}$
(4.98)forward	-2	1	0	0	0	0
(4.98)backward	2	-1	0	0	0	0
(4.99)forward	0	-1	-1	1	0	0
(4.99)backward	0	1	1	-1	0	0
(4.100)forward	0	-1	0	-1	1	0
(4.100)backward	0	1	0	1	-1	0
(4.101)forward	0	-1	0	0	-1	1
(4.101)backward	0	1	0	0	1	-1
(4.102)	-1	0	0	0	0	0
(4.103)	1	0	0	0	0	0
(4.104)	1	0	0	0	0	0

Table 4.1: State Vector Change Table: The state of the system at any point in time is characterized by a state vector S. Its elements change when chemical reactions occur.

state of the system is characterized as a vector:

$$S = \begin{bmatrix} \mathcal{M} \\ \mathcal{D} \\ \mathcal{O}_{R_0} \\ \mathcal{O}_{R_1} \\ \mathcal{O}_{R_2} \\ \mathcal{O}_{R_3} \end{bmatrix} \tag{4.105}$$

Each element of the state vector S represents the number of molecules of that species. When a chemical reaction occurs, the number of molecules of each specie change and they are summarized in the state vector change table 4.1. The Gillespie algorithm [9, 10, 11] is widely used to simulate stochastic chemical reactions. In this work I use the Next Reaction algorithm developed by Gilbson and Bruck [10]. The simulation requires the following definitions:

Propensity a_i: The propensity a_i is the rate of changing S due to reaction i.

For example the propensity for the forward reaction of (4.98) is:

$$a_{1,f} = \frac{k_1}{\Omega}\mathcal{M}(\mathcal{M} - 1) \tag{4.106}$$

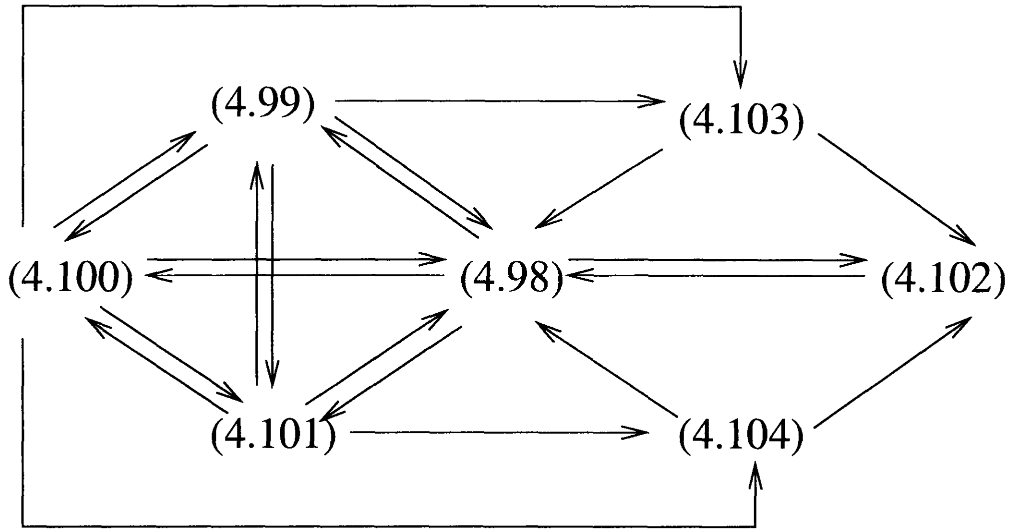

Figure 4-7: Dependency Graph: Each chemical reaction is denoted as a node and the influence of one node i to another node j is indicated as an arrow pointing from i to j.

Similarly the propensity for the backward reaction of (4.98) is

$$a_{1,b} = \theta_1 k_1 \mathcal{D} \tag{4.107}$$

The propensities for other reactions can be written in the same way.

Putative Time τ_i: The putative time τ_i for reaction i is a random time which follows the exponential distribution:

$$P(\tau_i)d\tau_i = a_i e^{-a_i \tau_i} d\tau_i \tag{4.108}$$

Physically, the putative time τ_i is the first passage time that reaction i will occur.

Dependency Graph: The graph that shows the influence of each reaction to others.

In a system of coupled chemical reactions, when a chemical reaction occurs it will change the state vector S and thus change the propensities and putative time for other reactions to which it couples. The dependency relations are drawn in the dependency graph. For the system in this appendix the dependency graph is shown in figure 4-7. It is important to point out that *each reaction also influences itself although this is not explicitly drawn in the* *dependency graph.*

The algorithm for the simulation is the following:

1. Initialization:

(a) set initial numbers of molecules to a state vector S, set $t \leftarrow 0$, draw a dependency graph $\mathscr{G}$;

(b) calculate the propensity a_i for each reaction i;

(c) generate a putative time τ_i for each reaction i according to (4.108) with parameter a_i;

(d) store the τ_i values in an indexed priority queue $\mathscr{P}$;

2. Find the reaction which has the least putative time in the $\mathscr{P}$ and denote this reaction as μ and its putative time τ_μ;

3. Set $\tau \leftarrow \tau_\mu$;

4. Look in the state vector change table and change S according to the entries of reaction μ. Set physically elapsed time $t \leftarrow \tau$;

5. For each reaction ν that is influenced by the reaction μ, which is indicated by an incoming arrow from μ in $\mathscr{G}$

(a) update a_ν;

(b) if $\nu \neq \mu$, set $\tau_\nu \leftarrow (a_{\nu,old}/a_{\nu,new})(\tau_\nu - t) + t$;

(c) If $\nu = \mu$, generate a random number ε, according to (4.108) with parameter a_μ and set $\tau_\mu \leftarrow \varepsilon + t$;

(d) replace the old τ_ν value in $\mathscr{P}$ with the new value;

6. Repeat the loop from 2.

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Chapter 5

Dynamic Phenotypic Switching: Influence of a Fluctuating Environment on Population Growth

Phenotypic switching is modelled dynamically as a problem of optimal phenotypic allocation under uncertainty. We discuss logarithmic fitness function and its generalization to power fitness functions. Based on our model and calculation, we propose a criterion for selecting between a responsive switching and a passive stochastic switching. We also calculate the dynamic long-term growth rate, i.e. Lyapunov exponent, without imposing ergodic conditions, to study how the information of an fluctuating environment is incorporated into the population growth. Further, we study the a complementary model in which sensing delay exists and we discuss how sensing delay could change the allocation probability. Finally we generalize the 2-phenotype model to a general M-phenotype model and discuss redundant phenotypes in phenotypic switching.

5.1 Introduction

Environmental conditions, such as temperature, illumination, number of resources and level of hazard etc., play an important role in the survival of organisms. The changes of environmental conditions are essentially stochastic and sometimes unpredictable. To study population survival in such a fluctuating environment, many mechanisms are proposed, e.g. adaptive mutations [1, 2], mutator phenotypes [3, 4, 5] and phase variation [6, 7] etc. Theoretical models for adaption to a fluctuating environment and optimal strategy for survival in a fluctuating environment have been built focusing on different regions of the problem. These include static mixed strategy and optimization in an ergodic fluctuating environment [8](Model 1), game theoretical based dynamic optimization in discrete time [9, 10, 11](Model 2) and a more recently proposed stochastic phenotypic switch and growth model in a fluctuating environment [12, 13, 14, 15](Model 3). Model 1 finds the static optimal strategy but suffers from an ergodic constraint. There is no ergodic assumption in model 2; however, the assumption of separated periods of decision making and population growth are made and a discrete time model is considered. Model 3 considers both responsive and stochastic switchings in continuous time where the environment is assumed to change slowly enough that for each environmental configuration the largest eigenvalue of the growth matrix is realized. Though model 3 in principle can be applied to a non-ergodic environment, the calculation for the Lyapunov exponents are restricted to an ergodic environment. For responsive switching, the optimal strategy in model 3 is to simply pick the phenotype that has the largest growth rate. We will show later that this is not always true and it depends on the fitness function. Besides the insights provided by these models, several important questions need to be answered in more detail, for example: How do organisms obtain the optimal strategy for population allocation in different phenotypes? How do they execute the optimal strategy? How do they decide whether to adopt an active or a passive strategy? Could there exist a redundancy in the number of phenotypes? To find suggestive answers to the above questions, we set up a continuous time model where the dynamics of the environment is used as an input and therefore there is no ergodic constraint. Within this model, we discuss the role of the fitness function and we find the dynamic optimal allocation strategy for 2-phenotype model for power and logarithmic fitness functions and thus calculate the Lyapunov exponents. We discuss the role of noise in adopting either passive stochastic switching or active responsive switching. Furthermore, we discuss the role of sensing delay on the optimal allocation strategy. Finally, we generalize the 2-phenotype case to the more general M-phenotype case, based on which we discuss the redundant phenotypes when phenotypic switching is used to hedge against environmental fluctuations.

5.2 2-phenotype model

The 2-phenotype model consists of a sensory machinery (SM) that acts as a social planner and two phenotypes. When the SM is active, it can probe some of the environmental conditions. This part of conditions is summarized as a random process $\mathcal{I}_t$:

$$d\mathcal{I}_t = \mu_I(\mathcal{I}_t)dt + \sigma_I(\mathcal{I}_t)dZ_{I,t} \tag{5.1}$$

where $Z_{I,t}$ is the standard Wiener process which describes the fluctuation of the probed part of the environment. The SM also observes the growth of each phenotype through the mechanism of feedback:

$$dn_{i,t} = r_i(n_{i,t}, \mathcal{I}_t)dt + \sigma_i(n_{i,t}, \mathcal{I}_t)dZ_{E,t}, \quad i = 1, 2 \tag{5.2}$$

where $n_{i,t}$ is the population of phenotype i at time t and r_i is the local deterministic growth rate of phenotype i at time t. σ_i is the influence of environmental fluctuations to phenotype i and $Z_{E,t}$ is a Wiener process describing the fluctuations of the entire environment. The correlation coefficient between the two processes $Z_{I,t}$ and $Z_{E,t}$ is

$$\rho = \mathbb{E}[Z_{I,t}Z_{E,t}]/\sqrt{\mathbb{E}[Z_{I,t}^2]\mathbb{E}[Z_{E,t}^2]} \in [-1, 1] \tag{5.3}$$

where $\mathbb{E}[\cdots]$ denotes expectation. So ρ has the interpretation of predictability of the probed part of the environment $\mathcal{I}_t$. Based on observations, the SM makes a decision on the optimal allocation probabilities $\{\phi_{i,t}\}$ to each phenotype. Here $\phi_{i,t}$ is the probability to switch to phenotype i at time t. This set of probabilities, serving as a control signal, is transmitted to individuals by mechanisms such as regulatory networks in which the message can be carried by regulatory proteins or chemicals. Each individual switches to phenotypes according to the probabilities contained in the control signal.

To determine $\{\phi_{i,t}\}$, the SM faces the problem of stochastic optimal control of population growth. To formulate this problem let N_t be the total population of organisms at time t. The SM maximizes a fitness function $f(N_t)$; however, the fitness function is generally unknown except that it must be a monotone increasing function. The most popularly used fitness function in modelling is the Lyapunov exponent[18, 8, 10]: $\frac{1}{T}\ln N_T$, which is related to the geometric mean of the overall growth rate. Generally speaking, the solution of a deterministic optimization problem is invariant under a nonlinear transformation $g(f(N_t))$ when $g(\cdot)$ is a monotone increasing function. However, this is no longer true for optimization under uncertainty as expectation does not commute with a nonlinear transformation:

$$\mathbb{E}\left[g(f(N_t))\right] \neq g(\mathbb{E}\left[f(N_t)\right]) \tag{5.4}$$

We generalize the log fitness function to a more general case for this problem:

$$U(N_t) = \frac{N_t^{1-\alpha} - 1}{1 - \alpha} \tag{5.5}$$

The logarithmic fitness function is a special case of this class: $\lim_{\alpha \to 1} U(N_t) = \ln N_t$. Given the stochastic process satisfied by each phenotype (5.2), we obtain a stochastic process for the total population:

$$dN_t = a(\Phi_t, N_t, \mathcal{I}_t)dt + b(\Phi_t, N_t, \mathcal{I}_t)dZ_{E,t} \tag{5.6}$$

where

$$a(\Phi_t, N_t, \mathcal{I}_t) = \sum_{i=1}^{2} r_i(\phi_{i,t} N_t, \mathcal{I}_t) \tag{5.7a}$$

$$b(\Phi_t, N_t, \mathcal{I}_t) = \sum_{i=1}^{2} \sigma_i(\phi_{i,t} N_t, \mathcal{I}_t) \tag{5.7b}$$

where

$$\Phi_t = \begin{bmatrix} \phi_{1,t} \\ \phi_{2,t} \end{bmatrix} \tag{5.8}$$

Notice that individuals switch to phenotypes according to the same set of probabilities, so $\phi_{i,t}$ is also the fraction of total population allocated to phenotype i at time t. Now we can formulate the SM's optimal strategy problem as:

$$\max_{\Phi_t} \mathbb{E}_0 \left[U(N_T) \right] \tag{5.9}$$

subject to

$$\sum_{i=1}^{2} \phi_{i,t} = 1 \tag{5.10a}$$

$$\phi_{i,t} \in [0, 1] \tag{5.10b}$$

and equations (5.1) and (5.6). Here $\mathbb{E}_0[\cdot]$ denotes expectation with respect to the probability law of the process N_t starting at N_0.

5.3 Optimal Allocation and the Selection between Responsive and Passive Phenotypic Switchings

The SM's optimal strategy problem can be solved using the dynamic programming techniques. Let $J(N_t, \mathcal{I}_t, t)$ be the value function defined as

$$J(N_t, \mathcal{I}_t, t) = \max_{\Phi_t} \mathbb{E}_t \left[U(N_T) \right] \tag{5.11}$$

Then $J(N_t, \mathcal{I}_t, t)$ solves the Hamilton-Jacobi-Bellman (HJB) equation:

$$\begin{aligned}\max_{\Phi_t} \quad \{ & \partial_t J + a(\Phi_t, N_t, \mathcal{I}_t)\partial_N J + \mu_I(\mathcal{I}_t)\partial_I J \\ + & \frac{1}{2}[b^2(\Phi_t, N_t, \mathcal{I}_t)\partial_N^2 J + \sigma_I^2(\mathcal{I}_t)\partial_I^2 J] \\ + & \rho\, b(\Phi_t, N_t, \mathcal{I}_t)\sigma_I(\mathcal{I}_t)\partial_{N,I}^2 J\} = 0\end{aligned} \tag{5.12}$$

with the boundary condition:

$$J(N_T, \mathcal{I}_T, T) = U(N_T) \tag{5.13}$$

We will examine the cases of power fitness function and logarithmic fitness function. In addition, we assume that each phenotype's population follows a geometric Brownian motion:

$$a(\Phi_t, N_t, \mathcal{I}_t) = N_t \Phi_t^T r(\mathcal{I}_t) \tag{5.14a}$$

$$b(\Phi_t, N_t, \mathcal{I}_t) = N_t \Phi_t^T \sigma(\mathcal{I}_t) \tag{5.14b}$$

Define

$$r(\mathcal{I}_t) = \begin{bmatrix} r_1(\mathcal{I}_t) \\ r_2(\mathcal{I}_t) \end{bmatrix} \tag{5.15a}$$

$$\sigma(\mathcal{I}_t) = \begin{bmatrix} \sigma_1(\mathcal{I}_t) \\ \sigma_2(\mathcal{I}_t) \end{bmatrix} \tag{5.15b}$$

The HJB equation for this case is

$$\begin{aligned}\max_{\Phi_t} \quad \{ & \partial_t J + N_t \Phi_t^T r(\mathcal{I}_t)\partial_N J + \mu_I(\mathcal{I}_t)\partial_I J \\ + & \frac{1}{2}[N_t^2 \Phi_t^T \sigma(\mathcal{I}_t)\sigma^T(\mathcal{I}_t)\Phi_t \partial_N^2 J + \sigma_I^2(\mathcal{I}_t)\partial_I^2 J] \\ + & \rho\, N_t \Phi_t^T \sigma(\mathcal{I}_t)\sigma_I(\mathcal{I}_t)\partial_{N,I}^2 J\} = 0\end{aligned} \tag{5.16}$$

5.3.1 Power Fitness Function

The power fitness function is defined in (5.5) as a generalization of logarithm fitness function. Let $\phi_t = \phi_{2,t}$, so $\phi_{1,t} = 1 - \phi_t$. The HJB equation (5.16) can be rewritten as a

$$\begin{aligned} \max_{\phi_t} \quad \{ & \partial_t J + N_t[r_1(\mathcal{I}_t) + \phi_t(r_2(\mathcal{I}_t) - r_1(\mathcal{I}_t))]\partial_N J + \mu_I(\mathcal{I}_t)\partial_I J \\ + & \frac{1}{2}[N_t^2[\sigma_1(\mathcal{I}_t) + \phi_t(\sigma_2(\mathcal{I}_t) - \sigma_1(\mathcal{I}_t))]^2 \partial_N^2 J + \sigma_I^2(\mathcal{I}_t)\partial_I^2 J] \\ + & \rho\ N_t[\sigma_1(\mathcal{I}_t) + \phi_t(\sigma_2(\mathcal{I}_t) - \sigma_1(\mathcal{I}_t))]\sigma_I(\mathcal{I}_t)\partial_{N,I}^2 J\} = 0 \end{aligned} \tag{5.17}$$

where ϕ_t is the allocation probability to phenotype 2. The first order condition gives ϕ_t as a function of $J(N_t, \mathcal{I}_t, t)$ and its derivatives:

$$\phi_t = -\frac{(r_2(\mathcal{I}_t) - r_1(\mathcal{I}_t))\partial_N J + \rho[\sigma_2(\mathcal{I}_t) - \sigma_1(\mathcal{I}_t)]\sigma_I(\mathcal{I}_t)\partial_{N,I}^2 J}{[\sigma_2(\mathcal{I}_t) - \sigma_1(\mathcal{I}_t)]^2 N_t \partial_N^2 J} - \frac{\sigma_1(\mathcal{I}_t)}{\sigma_2(\mathcal{I}_t) - \sigma_1(\mathcal{I}_t)} \tag{5.18}$$

Notice $\partial_N^2 J < 0$ since J is a concave increasing function. Substitute the expression (5.18) for ϕ_t to HJB equation (5.17) we obtain a nonlinear differential equation for J:

$$\begin{aligned} & \partial_t J + N_t r_1(\mathcal{I}_t)\partial_N J + \mu_I(\mathcal{I}_t)\partial_I J + \frac{1}{2}(\sigma_I^2(\mathcal{I}_t)\partial_I^2 J + N_t^2 \sigma_1(\mathcal{I}_t)^2 \partial_N^2 J) + \rho N_t \sigma_1(\mathcal{I}_t)\sigma_I(\mathcal{I}_t)\partial_{N,I}^2 J \\ & - \frac{[(r_2(\mathcal{I}_t) - r_1(\mathcal{I}_t))\partial_N J + (\sigma_2(\mathcal{I}_t) - \sigma_1(\mathcal{I}_t))(\rho\sigma_I(\mathcal{I}_t)\partial_{N,I}^2 J + N_t \sigma_1(\mathcal{I}_t)\partial_N^2 J)]^2}{2[\sigma_2(\mathcal{I}_t) - \sigma_1(\mathcal{I}_t)]^2 \partial_N^2 J} = 0 \end{aligned} \tag{5.19}$$

Without losing generality, we can assume that phenotype 1 has a smaller instantaneous growth rate than phenotype 2: $r_1(\mathcal{I}_t) < r_2(\mathcal{I}_t)$. If phenotype 1 also has higher fluctuation $\sigma_1(\mathcal{I}_t) > \sigma_2(\mathcal{I}_t)$, it can be seen from equation (5.18) that switching to phenotype 1 is not optimal. This is intuitively easy to understand as SM would choose a phenotype that has a high growth rate and a low fluctuation amplitude when the environment changes. In this case SM will switch to phenotype 2 almost surely. To exclude this trivial case, I assume $\sigma_1(\mathcal{I}_t) \ll \sigma_2(\mathcal{I}_t)$. In this case though the phenotype 1 has a smaller growth rate, it nevertheless is very stable against environmental changes. In the following derivation for optimal phenotypic switch in a fluctuating environment, I will assume $\sigma_1(\mathcal{I}_t) = 0$.

Under the above simplification, equation (5.19) becomes

$$\begin{aligned}&\partial_t J + N_t r_1(\mathcal{I}_t)\partial_N J + \mu_I(\mathcal{I}_t)\partial_I J + \frac{1}{2}\sigma_I^2(\mathcal{I}_t)\partial_I^2 J \\ &-\frac{[(r_2(\mathcal{I}_t) - r_1(\mathcal{I}_t))\partial_N J + \rho\sigma_2(\mathcal{I}_t)\sigma_I(\mathcal{I}_t)\partial_{N,I}^2 J]^2}{2\sigma_2^2(\mathcal{I}_t)\partial_N^2 J} = 0\end{aligned} \tag{5.20}$$

The initial condition for J is

$$J(N_T, \mathcal{I}_T, T) = \frac{N_T^{1-\alpha}}{1-\alpha} \tag{5.21}$$

So we look for a solution in the following form:

$$J(N_t, \mathcal{I}_t, t) = \left(\frac{N_t^{1-\alpha}}{1-\alpha}\right) f(\mathcal{I}_t, t) \tag{5.22}$$

where the unknown function $f(\mathcal{I}_t, t)$ satisfies an initial condition $f(\mathcal{I}_T, T) = 1$. Substituting (5.22) into (5.19) we obtain

$$\begin{aligned}&\partial_t f + (1-\alpha) r_1(\mathcal{I}_t) f + \mu_I(\mathcal{I}_t)\partial_I f + \frac{1}{2}\sigma_I^2(\mathcal{I}_t)\partial_I^2 f \\ &+\frac{(1-\alpha)[(r_2(\mathcal{I}_t) - r_1(\mathcal{I}_t)) f + \rho\sigma_2(\mathcal{I}_t)\sigma_I(\mathcal{I}_t)\partial_I f]^2}{2\alpha\sigma_2^2(\mathcal{I}_t) f} = 0\end{aligned} \tag{5.23}$$

Let

$$f(\mathcal{I}_t, t) = \exp[g(\mathcal{I}_t, t)] \tag{5.24}$$

Then the nonlinear differential equation (5.23) becomes

$$\begin{aligned}&\partial_t g + (1-\alpha) r_1(\mathcal{I}_t) + \mu_I(\mathcal{I}_t)\partial_I g + \frac{1}{2}\sigma_I^2(\mathcal{I}_t)[(\partial_I g)^2 + \partial_I^2 g] \\ &+\frac{(1-\alpha)[r_2(\mathcal{I}_t) - r_1(\mathcal{I}_t) + \rho\sigma_2(\mathcal{I}_t)\sigma_I(\mathcal{I}_t)\partial_I g]^2}{2\alpha\sigma_2^2(\mathcal{I}_t)} = 0\end{aligned} \tag{5.25}$$

I will look for a solution to (5.25) in the following form:

$$g(\mathcal{I}_t, t) = A(t)\mathcal{I}_t^2 + B(t)\mathcal{I}_t + C(t) \tag{5.26}$$

where the three unknown functions $A(t)$, $B(t)$ and $C(t)$ satisfy the initial condition: $A(T) = B(T) = C(T) = 0$. Up to now, the framework is quite general. To determine $A(t)$, $B(t)$ and $C(t)$ I will study the following model:

$$r_1(\mathcal{I}_t) = r_1 \tag{5.27a}$$

$$r_2(\mathcal{I}_t) = r_2 + s\mathcal{I}_t \tag{5.27b}$$

$$\sigma_2(\mathcal{I}_t) = \sigma_2 \tag{5.27c}$$

$$\mu_I(\mathcal{I}_t) = -k\mathcal{I}_t \tag{5.27d}$$

$$\sigma_I(\mathcal{I}_t) = \sigma_I \tag{5.27e}$$

This model describes the following situation: The part of environmental conditions being probed, $\mathcal{I}_t$, follows an Ornstein-Uhlenbeck process with a reverting force proportional to k. Phenotype 1 grows at a stable rate r_1 and it is not affected by environmental changes. Phenotype 2 has an instantaneous growth rate $r_2 + s\mathcal{I}_t$. The sensitivity of its growth rate to changes in $\mathcal{I}_t$ is characterized by parameter s. If $s > 0$ then phenotype 2 grows fast in "good" periods but it suffers or even dies during "bad" periods. For this particular model, substituting (5.26) and (5.27) to (5.25) and we get

$$\begin{aligned}&\dot{A}\mathcal{I}_t^2 + \dot{B}\mathcal{I}_t + \dot{C} + (1-\alpha)r_1 - k\mathcal{I}_t(2A\mathcal{I}_t + B) + \frac{1}{2}\sigma_I^2[(2A\mathcal{I}_t + B)^2 + 2A] \\ &+ \frac{(1-\alpha)[s\mathcal{I}_t + r_2 - r_1 + \rho\sigma_2\sigma_I(2A\mathcal{I}_t + B)]^2}{2\alpha\sigma_2^2} = 0\end{aligned} \tag{5.28}$$

This is a polynomial equation for $\mathcal{I}_t$ and it has to hold for every $\mathcal{I}_t$, so all coefficients of the polynomial should vanish identically. This leads to the following ODEs for $A(t)$, $B(t)$ and $C(t)$:

$$\dot{A} + 2\sigma_I^2\left(1 + \frac{(1-\alpha)\rho^2}{\alpha}\right)A^2 + 2\left(\frac{s(1-\alpha)\rho\sigma_I}{\alpha\sigma_2} - k\right)A + \frac{(1-\alpha)s^2}{2\alpha\sigma_2^2} = 0 \tag{5.29a}$$

$$\dot{B} + \left(\frac{\rho\sigma_I(1-\alpha)(s + 2\rho\sigma_2\sigma_I A)}{\alpha\sigma_2} + 2\sigma_I^2 A - k \right) B + \frac{(1-\alpha)(r_2 - r_1)(s + 2\rho\sigma_2\sigma_I A)}{\alpha\sigma_2^2} = 0 \tag{5.29b}$$

$$\dot{C} + (1-\alpha)r_1 + \frac{1}{2}\sigma_I^2(2A + B^2) + \frac{(1-\alpha)(r_2 - r_1 + \rho\sigma_2\sigma_I B)^2}{2\alpha\sigma_2^2} = 0 \tag{5.29c}$$

ODEs (5.29) are straightforward to solve though the final expressions are tedious. We will not list them here. Having solved the HJB equation we finally obtain the optimal allocation probability for phenotype 2:

$$\phi_t = \frac{r_2 - r_1 + s\mathcal{I}_t + \rho\sigma_2\sigma_I[2A(t)\mathcal{I}_t + B(t)]}{\alpha\sigma_2^2} \tag{5.30}$$

The optimal allocation probability for phenotype 2, ϕ_t, is proportional to its excess growth rate to the phenotype 1, $r_2 - r_1$, and it is inversely proportional to its exposure, σ_2, to the environmental fluctuation $Z_{\mathrm{E},t} \equiv \rho dZ_{1,t} + \sqrt{1-\rho^2}dZ_{2,t}$. Due to the nonlinearity of fitness function, ϕ_t is inversely proportional to parameter α. In the case when SM only cares about the expected population $\mathbb{E}[N_T]$, we have $\alpha = 0$ and $\phi_t \in \{0, 1\}$ which depends on the sign of the numerator in (5.30). This is easy to understand since the SM only has to choose the phenotype that has the largest instantaneous growth rate with probability one. This situation is considered recently by Kussell *et.al.*[15, 14]. When $\alpha \neq 1$, ϕ_t is reduced so that the SM would assign a nonzero probability to the slow but stable growing phenotype 1. Therefore α measures the risk averseness of the SM. This interpretation has a wide application in finance [19]. The time dependent part has two resources: (1)Instantaneous growth rate of phenotype 2 in response to the probed environment conditions, i.e. $s\mathcal{I}_t$; (2)Predictability of the information gathered, $\mathcal{I}_t$, to the whole environmental conditions which is measured by parameter ρ. If $\rho > 0$ then a good period of the probed environment $\mathcal{I}_t$, predicts a good period of the entire environment. In this case the SM would assign a higher probability to the phenotype 2 when $\mathcal{I}_t > 0$ and smaller probability when $\mathcal{I}_t < 0$. If $\rho < 0$ then a good period of the probed environment predicts a bad period of the entire environment. In this case there is a competition between the probed environment and the entire environment on the allocation probability to phenotype 2.

The time dependent part of ϕ_t indicates a necessity for responsive switching. This is intuitive as the more information gathered of the environment the higher the chance to survive. Nevertheless, sometimes responsive switching is not adopted. As is shown in recently research on noise propagation in gene networks[20, 21, 22], there exists intrinsic noise in regulatory gene networks due to the small size effect. So in the case where the observations of s are very noisy and $\mathcal{I}_t$ is not predicative, $\rho = 0$, for the entire environment, then the SM would simply adopt a time independent passive switching strategy:

$$\phi_t = \frac{r_2 - r_1}{\alpha \sigma_2^2} \tag{5.31}$$

In such a case the sensor machinery is turned off. Our analysis for choosing between a responsive and a passive switching mechanisms provides an additional criterion to the existing one which uses an argument of sensing cost[15].

5.3.2 Logarithmic Fitness Function

The logarithmic fitness function is popularly used in study of population growth [8, 10]. It corresponds to the geometric mean of growth rate and it is closely related to the Lyapunov exponent. As will be shown below it is a special case of the power fitness function(5.5). Since the stochastic optimization for the logarithmic fitness function is easy to solve we can remove the simplifying assumption made in the last section and consider a general case. The total population N_t follows the process

$$dN_t = N_t[r_1(\mathcal{I}_t) + \phi_t(r_2(\mathcal{I}_t) - r_1(\mathcal{I}_t))]dt + N_t[\sigma_1(\mathcal{I}_t) + \phi_t(\sigma_2(\mathcal{I}_t) - \sigma_1(\mathcal{I}_t))]dZ_{E,t} \tag{5.32}$$

where ϕ_t is the allocation probability for phenotype 2. From Ito's lemma we obtain

$$\ln N_T = \ln N_0 + \int_0^T dt P(\phi_t, \mathcal{I}_t) + \int_0^T dZ_{E,t} Q(\phi_t, \mathcal{I}_t) \tag{5.33}$$

where

$$P(\phi_t, \mathcal{I}_t) = r_1(\mathcal{I}_t) + \phi_t[r_2(\mathcal{I}_t) - r_1(\mathcal{I}_t)] - \frac{1}{2}[\sigma_1(\mathcal{I}_t) + \phi_t(\sigma_2(\mathcal{I}_t) - \sigma_1(\mathcal{I}_t))]^2 \tag{5.34a}$$

$$Q(\phi_t, \mathcal{I}_t) = \sigma_1(\mathcal{I}_t) + \phi_t[\sigma_2(\mathcal{I}_t) - \sigma_1(\mathcal{I}_t)] \tag{5.34b}$$

Notice

$$\mathbb{E}_0[\int_0^T dZ_{E,t} Q(\phi_t, \mathcal{I}_t)] = 0$$

Therefore the optimization problem becomes

$$\begin{aligned} & \max_{\phi_t} \mathbb{E}_0[\ln N_T] \\ = \; & \ln N_0 + \max_{\phi_t} \mathbb{E}_0[\int_0^T dt P(\phi_t, \mathcal{I}_t)] \end{aligned} \tag{5.35}$$

ϕ_t is obtained from the first order condition:

$$\partial_{\phi_t} P(\phi_t, \mathcal{I}_t) = 0$$

So we get the optimal allocation probability to phenotype 2:

$$\phi_t = \frac{r_2(\mathcal{I}_t) - r_1(\mathcal{I}_t)}{[\sigma_2(\mathcal{I}_t) - \sigma_1(\mathcal{I}_t)]^2} - \frac{\sigma_1(\mathcal{I}_t)}{\sigma_2(\mathcal{I}_t) - \sigma_1(\mathcal{I}_t)} \tag{5.36}$$

For the logarithmic fitness function, we see that the predictability of $\mathcal{I}_t$ for the entire environment is not relevant to the optimal allocation probability and there is no hedging probability assigned for this predictability. ϕ_t is determined purely from the instantaneous growth rate and exposure to environmental fluctuations: it is proportional to the instantaneous excess growth rate of phenotype 2 and it is inversely proportional to the phenotype 2's excess exposure to the environmental fluctuations. If we impose the same simplification as the last section: $\sigma_1(\mathcal{I}_t) = 0$, (5.36) gives the same result as (5.30) ($\alpha = 1, A(t) = B(t) = 0$), so the logarithmic fitness function is indeed a special case of the power fitness function. Therefore it is useful to consider a much large class of nonlinear fitness functions to study the problem of phenotypic switching in a fluctuating environment.

For the SM that adopts a logarithmic fitness function, it is profitable to use responsive switching only if the noise in observing the functional relationship between phenotype growth and the probed environmental conditions is below a certain threshold level. If there is a prevailing intrinsic noise in the regulatory and feedback gene networks, passive switching will be adopted no matter how strong the predictability of $\mathcal{I}_t$ is.

5.4 Lyapunov Exponent

In this section we will discuss how the information of the fluctuating environment is encoded in the phenotypic growth. It is clear that the optimal allocation probability ϕ_t, (5.30) and (5.36), contains such information. Another measure discussed in the literature is the Lyapunov exponent, which is related to the geometric mean of long-term growth rate:

$$\Lambda_T = \frac{1}{T} \ln N_T \tag{5.37}$$

In a fluctuating environment, the Lyapunov exponent is no longer a deterministic quantity but a functional of the entire environment. Using Ito's lemma (see appendix A)it can be written in the following form:

$$\Lambda_T[\mathcal{I}_t] = \frac{1}{T} \ln N_0 + \frac{1}{T} \int_0^T dtR(\mathcal{I}_t) + \frac{1}{T} \int_0^T dZ_{E,t} V(\mathcal{I}_t) \tag{5.38}$$

The first term is a residual term arising from initial condition and it goes to zero as $T \to \infty$. The second term shows the influence of the probed part of environment $\mathcal{I}_t$ on the average long-term growth rate. The third term is the influence of the entire environmental fluctuation. Since (5.32) holds generally for both the power fitness function and the logarithmic fitness function we obtain:

$$R(\mathcal{I}_t) = \sum_{i=1}^{2} \phi_{i,t}(\mathcal{I}_t) r_{i,t}(\mathcal{I}_t) - \frac{1}{2}\left(\sum_{i=1}^{2} \phi_{i,t}(\mathcal{I}_t)\sigma_{i,t}(\mathcal{I}_t)\right)^2 \tag{5.39a}$$

$$V(\mathcal{I}_t) = \sum_{i=1}^{2} \phi_{i,t}(\mathcal{I}_t)\sigma_{i,t}(\mathcal{I}_t) \tag{5.39b}$$

where $\phi_{i,t}(\mathcal{I}_t)$ is the optimal allocation probability for phenotype i. For phenotype 2, $\phi_{2,t}$ is given by (5.30) and (5.36), while $\phi_{1,t} = 1 - \phi_{2,t}$. Notice that $R(\mathcal{I}_t)$ has two contributions: the first one is the sum of instantaneous growth rate of each phenotype weighted by its optimal allocation probability; the second contribution comes from the Ito correction which reduces the Lyapunov exponent. This additional term missing from a deterministic environment can be interpreted as a hedging against uncertainty.

5.5 Sensing Delay

In section 5.3 we considered the case when SM is able to optimize at every point in time and the strategy is carried out by individuals almost immediately. This is a good approximation if the environment stays long enough in each of its configuration such that the actions can be completed. In this section we will consider a complementary case. Namely the environment cannot stay long enough for the decision-making and strategy-executing to be completed.

For simplicity I consider two phenotypes and logarithmic fitness function. I assume that on average it takes τ for the signal to be transmitted and executed, so τ is a parameter characterizing sensing delay. The total population N_t then follows the process:

$$dN_t = N_t[r_1(\mathcal{I}_t) + \phi_{t-\tau}(r_2(\mathcal{I}_t) - r_1(\mathcal{I}_t))]dt + N_t[\sigma_1(\mathcal{I}_t) + \phi_{t-\tau}(\sigma_2(\mathcal{I}_t) - \sigma_1(\mathcal{I}_t))]dZ_{E,t} \tag{5.40}$$

The optimization problem becomes:

$$\begin{aligned}
& \max_{\phi_t} \mathbb{E}_0[\ln N_T] \\
= \; & \ln N_0 + \int_0^{\tau} dt \left(r_1(\mathcal{I}_t) + \phi_{t-\tau}[r_2(\mathcal{I}_t) - r_1(\mathcal{I}_t)] - \frac{1}{2}[\sigma_1(\mathcal{I}_t) + \phi_{t-\tau}(\sigma_2(\mathcal{I}_t) - \sigma_1(\mathcal{I}_t))]^2 \right) \\
+ \; & \max_{\phi_t} \mathbb{E}_0[\int_{\tau}^{T} dt \left(r_1(\mathcal{I}_t) + \phi_{t-\tau}[r_2(\mathcal{I}_t) - r_1(\mathcal{I}_t)] - \frac{1}{2}[\sigma_1(\mathcal{I}_t) + \phi_{t-\tau}(\sigma_2(\mathcal{I}_t) - \sigma_1(\mathcal{I}_t))]^2 \right)]
\end{aligned}$$

which follows from the fact that ϕ_t is $\mathcal{F}_t$-measurable, where $\mathcal{F}_t$ is a filtration on probability space $(\Omega, \mathcal{F}, P)$, so ϕ_t is known for $t < 0$. We only have to maximize the last term:

$$\begin{aligned}
\max_{\phi_t} \mathbb{E}_0[\quad & \int_0^{T-\tau} dt(\; r_1(\mathcal{I}_{t+\tau}) + \phi_t[r_2(\mathcal{I}_{t+\tau}) - r_1(\mathcal{I}_{t+\tau})] \\
& -\frac{1}{2}[\sigma_1(\mathcal{I}_{t+\tau}) + \phi_t(\sigma_2(\mathcal{I}_{t+\tau}) - \sigma_1(\mathcal{I}_{t+\tau}))]^2) \;]
\end{aligned} \tag{5.41}$$

by a changing of integration variable. We look for a control ϕ_t of the following form:

$$\phi_t = \sum_{i=0}^{m-1} \phi_{t_i} \chi_{(t_i, t_{i+1}]}(t) \tag{5.42}$$

where $\mathcal{P}_m = \{0 = t_0 < t_1 < \cdots < t_{m-1} < t_m = T - \tau\}$ is a sequence of partition and suppose that $\lim_{m \to \infty} \delta(\mathcal{P}_m) = 0$, where the mesh $\delta(\mathcal{P}_m) = \max_{0 \le i \le m-1} |t_{i+1} - t_i|$. ϕ_{t_i} is a $\mathcal{F}_{t_i}$-measurable function and $\chi_{(t_i, t_{i+1}]}(t)$ is an indicator function:

$$\chi_{(t_i, t_{i+1}]}(t) = \begin{cases} 1 & \text{if } t \in (t_i, t_{i+1}], \\ 0 & \text{if } t \notin (t_i, t_{i+1}]. \end{cases} \tag{5.43}$$

The ϕ_t, being a simple function, corresponds to a situation where the SM adopts a strategy for a period of time and then changes it to new one for another period of time.

Substituting (5.42) to (5.41) we obtain:

$$\begin{aligned}\max_{\phi_{t_i}} \mathbb{E}_0[\quad & \int_0^{T-\tau} dt(r_1(\mathcal{I}_{t+\tau}) - \frac{1}{2}\sigma_1^2(\mathcal{I}_{t+\tau})) + \sum_{i=0}^{m-1} \phi_{t_i}\mathbb{E}_{t_i}[\int_{t_i}^{t_{i+1}} dt\,(r_2(\mathcal{I}_{t+\tau}) - r_1(\mathcal{I}_{t+\tau}))] \\ & - \sum_{i=0}^{m-1} \phi_{t_i}\mathbb{E}_{t_i}[\int_{t_i}^{t_{i+1}} dt\;\sigma_1(\mathcal{I}_{t+\tau})(\sigma_2(\mathcal{I}_{t+\tau}) - \sigma_1(\mathcal{I}_{t+\tau}))] \\ & - \frac{1}{2}\sum_{i=0}^{m-1} \phi_{t_i}^2\mathbb{E}_{t_i}[\int_{t_i}^{t_{i+1}} dt\;(\sigma_2(\mathcal{I}_{t+\tau}) - \sigma_1(\mathcal{I}_{t+\tau}))^2] \\ ] \quad & \end{aligned} \tag{5.44}$$

where we have used the property of iterated expectation. Taking the limit $m \to \infty$ we find

$$\begin{aligned}\max_{\phi_t} \mathbb{E}_0[\quad & \int_0^{T-\tau} dt\;(r_1(\mathcal{I}_{t+\tau}) - \frac{1}{2}\sigma_1^2(\mathcal{I}_{t+\tau})) + \int_0^{T-\tau} dt\;\phi_t\mathbb{E}_t[r_2(\mathcal{I}_{t+\tau}) - r_1(\mathcal{I}_{t+\tau})] \\ & - \int_0^{T-\tau} dt\;\phi_t\mathbb{E}_t[\sigma_1(\mathcal{I}_{t+\tau})(\sigma_2(\mathcal{I}_{t+\tau}) - \sigma_1(\mathcal{I}_{t+\tau}))] \\ & - \frac{1}{2}\int_0^{T-\tau} dt\;\phi_t^2\mathbb{E}_t[(\sigma_2(\mathcal{I}_{t+\tau}) - \sigma_1(\mathcal{I}_{t+\tau}))^2] \\ ] \quad & \end{aligned} \tag{5.45}$$

Therefore the optimal allocation probability to phenotype 2 is:

$$\phi_t = \frac{\mathbb{E}_t[r_2(\mathcal{I}_{t+\tau}) - r_1(\mathcal{I}_{t+\tau})] - \mathbb{E}_t[\sigma_1(\mathcal{I}_{t+\tau})(\sigma_2(\mathcal{I}_{t+\tau}) - \sigma_1(\mathcal{I}_{t+\tau}))]}{\mathbb{E}_t[(\sigma_2(\mathcal{I}_{t+\tau}) - \sigma_1(\mathcal{I}_{t+\tau}))^2]} \tag{5.46}$$

Now we will discuss the effect of sensing delay and in particular we would like to answer the question: How would the SM change the allocation probability of the fast growing phenotype (phenotype 2) comparing to the case where there exists no sensing delay? First consider the case where the phenotypes' exposures to the fluctuation of the entire environment are independent of $\mathcal{I}_t$. If the excess growth rate of fast growing phenotype is a convex function of $\mathcal{I}_t$, then we have

$$\phi_t \geq \frac{r_2(\mathbb{E}_t[\mathcal{I}_{t+\tau}]) - r_1(\mathbb{E}_t[\mathcal{I}_{t+\tau}]) - \sigma_1(\sigma_2 - \sigma_1)}{(\sigma_2 - \sigma_1)^2} \tag{5.47}$$

by Jensen's inequality (see appendix A). The equality holds when $r_2(\mathcal{I}_t)$ and $r_1(\mathcal{I}_t)$ are linear in $\mathcal{I}_t$. We find that if $\mathcal{I}_t$ is a submartingale then the SM will increase the allocation probability to the fast growing phenotype. This means that when the expected future environmental condition $\mathcal{I}_{t+\tau}$ is better than today's, more allocation probability will be given to the present fast growing phenotype compared to no sensing delay. On the other hand if $\mathcal{I}_t$ is a supermartingale and if the excess growth rate $r_2(\mathcal{I}_t) - r_1(\mathcal{I}_t)$ is a linear function of $\mathcal{I}_t$ then

$$\begin{aligned}\phi_t &= \frac{r_2(\mathbb{E}_t[\mathcal{I}_{t+\tau}]) - r_1(\mathbb{E}_t[\mathcal{I}_{t+\tau}]) - \sigma_1(\sigma_2 - \sigma_1)}{(\sigma_2 - \sigma_1)^2} \\ &\leq \frac{r_2(\mathcal{I}_t) - r_1(\mathcal{I}_t) - \sigma_1(\sigma_2 - \sigma_1)}{(\sigma_2 - \sigma_1)^2} \end{aligned} \tag{5.48}$$

In this case, the expected future environmental condition $\mathcal{I}_{t+\tau}$ is worse than today's so less allocation probability will be assigned to the fast growing phenotype.

Second, we consider the case when phenotypes' exposures to the entire environmental fluctuations depend on the probed environmental condition $\mathcal{I}_t$ and we assume $\sigma_1(\mathcal{I}_t) = 0$:

$$\phi_t = \frac{\mathbb{E}_t[r_2(\mathcal{I}_{t+\tau}) - r_1(\mathcal{I}_{t+\tau})]}{\mathbb{E}_t[\sigma_2^2(\mathcal{I}_{t+\tau})]} \tag{5.49}$$

If $\mathcal{I}_t$ is a martingale(see appendix A), the excess growth rate is a linear function of $\mathcal{I}_t$ and if $\sigma_2(\mathcal{I}_t)$ is a linear or convex function of $\mathcal{I}_t$ then

$$\begin{aligned}\phi_t &= \frac{r_2(\mathbb{E}_t[\mathcal{I}_{t+\tau}]) - r_1(\mathbb{E}_t[\mathcal{I}_{t+\tau}])}{\mathbb{E}_t[\sigma_2^2(\mathcal{I}_{t+\tau})]} \\ &\leq \frac{r_2(\mathbb{E}_t[\mathcal{I}_{t+\tau}]) - r_1(\mathbb{E}_t[\mathcal{I}_{t+\tau}])}{\sigma_2^2(\mathbb{E}_t[\mathcal{I}_{t+\tau}])} \\ &= \frac{r_2(\mathcal{I}_t) - r_1(\mathcal{I}_t)}{\sigma_2^2(\mathcal{I}_t)} \end{aligned} \tag{5.50}$$

We find that even if the expectation of future environmental condition $\mathcal{I}_{t+\tau}$ is the same as today's, the SM will decrease the allocation probability to the fast growing phenotype compared to no sensing delay. This shows that sensing delay brings in uncertainties about future environmental conditions such that less probability is given to the fast but vulnerable phenotype to hedge against that. If $\mathcal{I}_t$ is a submartingale, the excess growth rate is a convex function of $\mathcal{I}_t$ and if $\sigma_2(\mathcal{I}_t)$ is a linear or convex function of $\mathcal{I}_t$ then

$$\mathbb{E}_t[r_2(\mathcal{I}_{t+\tau}) - r_1(\mathcal{I}_{t+\tau})] \geq r_2(\mathcal{I}_t) - r_1(\mathcal{I}_t) \tag{5.51a}$$

$$\mathbb{E}_t[\sigma_2^2(\mathcal{I}_{t+\tau})] \geq \sigma_2^2(\mathbb{E}_t[\mathcal{I}_{t+\tau}]) \geq \sigma_2^2(\mathcal{I}_t) \tag{5.51b}$$

In this case there are two competing factors: expected improvement in the excess growth rate and expected larger exposure to environmental fluctuations caused by sensing delay. So the change of allocation probability for the fast growing phenotype depends on the relative strength of the two factors.

5.6 M-phenotype and Phenotypic Redundancy

In this section, we will generalize the treatment of two-phenotype to M-phenotype. If we simply extend two-phenotype to M-phenotype in the following way:

$$dn_{i,t} = r_i(n_{i,t}, \mathcal{I}_t)dt + \sigma_i(n_{i,t}, \mathcal{I}_t)dZ_{E,t}, \quad i = 1, \cdots, M \tag{5.52}$$

it is clear that the first order condition for the HJB equation (5.16) generally does not have a solution. This is because $\sigma(\mathcal{I}_t)\sigma(\mathcal{I}_t)^T$ is a projection matrix, where

$$\sigma(\mathcal{I}_t) = (\sigma_1(\mathcal{I}_t), \cdots, \sigma_M(\mathcal{I}_t))^T \tag{5.53}$$

so it is not invertible. We shall explain this mathematical 'difficulty' as being caused by phenotypic redundancy. As a general case, we consider the following model

$$\begin{aligned} dn_{1,t} &= n_{1,t}r_1(\mathcal{I}_t)dt + n_{1,t}\sum_{j=1}^{L}\sigma_{1,j}(\mathcal{I}_t)dZ_{E,t}^j \\ &= N_t(1 - \sum_{i=2}^{M}\phi_{i,t})r_1(\mathcal{I}_t)dt + N_t(1 - \sum_{i=2}^{M}\phi_{i,t})\sum_{j=1}^{L}\sigma_{1,j}(\mathcal{I}_t)dZ_{E,t}^j \end{aligned} \tag{5.54a}$$

$$\begin{aligned} dn_{i,t} &= n_{i,t} r_i(\mathcal{I}_t)dt + n_{i,t} \sum_{j=1}^{L} \sigma_{i,j}(\mathcal{I}_t) dZ_{E,t}^j \\ &= N_t \phi_{i,t} r_i(\mathcal{I}_t)dt + N_t \phi_{i,t} \sum_{j=1}^{L} \sigma_{i,j}(\mathcal{I}_t) dZ_{E,t}^j \quad i = 2, \cdots, M \end{aligned} \tag{5.54b}$$

$\Phi_t = (\phi_{2,t}, \cdots, \phi_{M,t})^T$ is the allocation probability vector, where $\phi_{i,t}$ is the allocation probability to phenotype i. The environmental fluctuation vector $Z_{E,t} = (Z_{E,t}^1, \cdots, Z_{E,t}^L)^T$ consists of L independent fluctuation components $Z_{E,t}^j$. The matrix element $\sigma_{i,j}$ is the exposure of the ith phenotype to the jth environmental fluctuation $Z_{E,t}^j$. The probed part of the environment $\mathcal{I}_t$ satisfies (5.1) and has a correlation vector $\varrho = (\rho_1, \cdots, \rho_L)^T$ where ρ_i is the correlation with the ith environmental fluctuation. Therefore the total population satisfies the following process:

$$dN_t = N_t r_{1,t} dt + N_t \sigma_{1,t}^T dZ_{E,t} + N_t \Phi_t^T \Delta r_t dt + N_t \Phi_t^T \Delta\sigma_t dZ_{E,t} \tag{5.55}$$

where

$$\sigma_{1,t} = \begin{bmatrix} \sigma_{1,1}(\mathcal{I}_t) \\ \vdots \\ \sigma_{1,L}(\mathcal{I}_t) \end{bmatrix} \tag{5.56}$$

and

$$r_t = \begin{bmatrix} r_2(\mathcal{I}_t) - r_1(\mathcal{I}_t) \\ \vdots \\ r_M(\mathcal{I}_t) - r_1(\mathcal{I}_t) \end{bmatrix} \tag{5.57}$$

is the excess growth rate vector. $\Delta\sigma_t^{ij} = \sigma_{i,j}(\mathcal{I}_t) - \sigma_{1,j}(\mathcal{I}_t)$ is excess exposure of the ith phenotype to the jth environmental fluctuation. The HJB equation is

$$\begin{aligned} \max_{\Phi_t} \quad \{ \quad & \partial_t J + N_t(r_{1,t} + \Phi_t^T \Delta r_t)\partial_N J + \mu_I(\mathcal{I}_t)\partial_I J \\ + \quad & \frac{1}{2} N_t^2 (\sigma_{1,t}^T + \Phi_t^T \Delta\sigma_t)(\sigma_{1,t} + \Delta\sigma_t^T \Phi_t)\partial_N^2 J \\ + \quad & \frac{1}{2}\sigma_I^2(\mathcal{I}_t)\partial_I^2 J + N_t(\sigma_{1,t}^T + \Phi_t^T \Delta\sigma_t)\varrho \partial_{N,I}^2 J\} = 0 \end{aligned} \tag{5.58}$$

The first order condition for this HJB equation is

$$\Delta\sigma_t\Delta\sigma_t^T\Phi_t = -\frac{\partial_N J}{N_t\partial_N^2 J}\Delta r_t - \frac{\partial_{N,I}^2 J}{N_t\partial_N^2 J}\Delta\sigma_t\varrho - \Delta\sigma_t\sigma_{1,t} \equiv Y \tag{5.59}$$

If $M-1 = L$ then $\Delta\sigma_t$ is a square matrix. If further $\text{Rank}([\Delta\sigma_t\Delta\sigma_t^T]) = \text{Rank}([\Delta\sigma_t\Delta\sigma_t^T|Y]) = M-1$, then $\Delta\sigma_t\Delta\sigma_t^T$ is an invertible matrix and we have

$$\Phi_t = (\Delta\sigma_t\Delta\sigma_t^T)^{-1}Y \tag{5.60}$$

which subjects to constraint $\phi_{i,t} \in [0,1]$ and $\sum_{i=2}^{M}\phi_{i,t} \leq 1$. In other words if the number of independent phenotypes, which are defined by conditions above, equals the number of independent environmental fluctuations plus one, then there exits a unique solution.

If $M-1 > L$ and $\text{Rank}([\Delta\sigma_t\Delta\sigma_t^T]) = \text{Rank}([\Delta\sigma_t\Delta\sigma_t^T|Y]) = L$, then the SM only needs to choose $L+1$ independent phenotypes out of total M phenotypes to solve optimization problem. We see in this case that there is a redundancy in the number of phenotypes to hedge environmental fluctuations.

If $M-1 > L$ and $\text{Rank}([\Delta\sigma_t\Delta\sigma_t^T]) \neq \text{Rank}([\Delta\sigma_t\Delta\sigma_t^T|Y])$, then the first order condition cannot be satisfied. The optimization problem has no interior solution and constrain $\phi_{i,t} = 0$ binds for some i. The optimal solution therefore exists in a subspace of M phenotypes. In fact, the solution is achieved by first selecting L independent phenotypes out of M phenotypes that solve the first order condition in this subspace. The optimal solution is the set of L independent phenotypes, among other sets, which maximizes the fitness function. In this case we also see redundancy of phenotypes to hedge environmental fluctuations.

If $M-1 < L$ and $\text{Rank}([\Delta\sigma_t\Delta\sigma_t^T]) = \text{Rank}([\Delta\sigma_t\Delta\sigma_t^T|Y]) = M-1$, then all phenotypes are needed to hedge the fluctuations of environment. However, this hedging is not complete and only $M-1$ out of L environmental fluctuations can be hedged. In this case there is insufficiency of phenotypes to hedge environmental fluctuations.

To summarize, we find that to hedge L independent environmental fluctuations completely, exactly $L+1$ independent phenotypes are needed. Our model therefore implies that in a real biological system the number of independent environmental fluctuations which are experienced by the biological system is equal to or larger than the number of existing phenotypes. In other words, in order to fully hedge L independent environmental fluctuations, equal number of independent phenotypes are necessary. However, redundant phenotypes do not improve the hedging against environmental fluctuations within our model and it might induce more sensing cost.

5.7 Conclusions

We studied phenotypic switching in a fluctuating environment in a continuous time model, where ergodic constraint is relaxed. In this model the SM can continuously probe part of of the entire environment and it can monitor the growth of each phenotype. Based on the information gathered, the SM sends out signals which consists of optimal phenotypic allocation probabilities for each phenotype. Since this optimization process in carried out under uncertainty, we showed that the optimal allocation probabilities depend on the form of the fitness function. For nonlinear fitness functions, we showed that it is not optimal to allocate population to the fastest growing phenotype with probability one. A fraction of population exist in a slow growing but stable phenotype to hedge against uncertainties. This principle of diversification also has wide application in financial economics.

We showed in both cases of the power fitness function and logarithmic fitness function that responsive switching is necessary to hedge against uncertainty while keeping an optimal growth rate. For the power fitness function, two factors come into play: predictability of the probed part of the environment $\mathcal{I}_t$ and excess growth rate of the fast phenotype. The SM can infer the global environmental conditions from the information gathered on the part of environmental that has a direct influence on the phenotypic growth rates. We showed that when the magnitude of noise (intrinsic and extrinsic) is so large that a definite relation between the probed environmental conditions and phenotypic growth rates cannot be obtained or when the probed part of environment is not predictive, it is possible that passive switching is adopted. In this case a static set of allocation probabilities is used and the SM can be turned off to reduce further sensing cost. For the logarithmic fitness function, the predictability of probed environmental conditions is irrelevant to the optimal allocation probabilities and sufficiently large noise in a regulatory network can make the SM choose passive stochastic switching. We also showed that in general the Lyapunov exponent is a functional of dynamics of the probed environmental conditions and the entire environmental fluctuations. An Itô correction term shows up in the expression of Lyapunov exponent indicating a hedging demand.

The above conclusions are reached in a model where there is no sensing delay which is a good approximation when the environment stays at a certain configuration long enough that the optimal strategy can form and be executed completely. We further showed that if there is a sensing delay then the set of optimal allocation probabilities will change. The change depends on the expected change of the probed part of the environment which has a direct influence on phenotypic growth rates. When the exposure of each phenotype to the fluctuation of the entire environment is a constant then the change of optimal allocation probabilities depends only on the possibility of an improved(or worsened) performance of $\mathcal{I}_{t+\tau}$. However, if the exposure to the total environmental fluctuations is also $\mathcal{I}_t$ dependent then there can exist a competition between improved environmental conditions $\mathcal{I}_{t+\tau}$ and larger exposure to global environmental fluctuations.

We finally discuss a general M-phenotype model. The conclusions for 2-phenotype model hold for the M-phenotype model: the mathematical structure of optimal allocation probabilities, the role of predictability of the probed part of the environment on optimal allocation probabilities and the role of noise on choice between responsive and passive phenotypic switchings etc. In addition we find that to fully hedge L independent global environmental fluctuations only L independent phenotypes are needed. Redundant phenotypes will not improve hedging against uncertainties within our model while fewer phenotypes cannot fully hedge against all environmental fluctuations.

5.8 Appendix A: Itô Calculus, Martingales and Diffusion Properties

5.8.1 Standard Brownian Motion Z

Mathematically, the standard Brownian motion Z is a stochastic process on a probability space $(\Omega, \mathcal{F}, P)$. It belongs to a general class of Lévy processes X. We say that a process has *independent increments* if for each $n \in \mathbb{N}$ and each $0 \leq t_1 \leq t_2 \leq \cdots \leq t_{n+1} < \infty$ the random variables $X(t_{j+1}) - X(t_j)$, $1 \leq j \leq n$ are independent. $X(t)$ has *stationary increments* if

$$X(t_{j+1}) - X(t_j) \overset{d}{=} X(t_{j+1} - t_j) + X(0) \tag{5.61}$$

where $\overset{d}{=}$ means equals in distribution. To simplify notations, I will use $X(t)$ and X_t interchangeably.

The standardBrownian motion Z satisfies the following conditions:

(1) $Z_0 = 0$ almost surely (a.s.);

(2) Z has independent and stationary increments;

(3) Z is stochastically continuous, i. e. for all $a > 0$ and all $s \geq 0$

$$\lim_{t \longrightarrow s} P(|Z_t - Z_s| > a) = 0 \tag{5.62}$$

The above conditions are satisfied by all Lévy processes. The standard Brownian motion must also satisfy the following conditions:

(4) $Z_t \sim N(0, t)$ for each $t \geq 0$;

(5) Z has continuous sample paths. $N(0, t)$ denotes the normal distribution with mean 0 and variance t which implies:

$$E[Z_t] = 0 \tag{5.63}$$

$$E\left[(Z_t - Z_s)^2\right] = t - s, \quad \text{for } t \geq s \tag{5.64}$$

5.8.2 Itô Integral and Itô's Lemma

Itô integral is defined as

$$\mathcal{I}[f](\omega) = \int_0^T f(t,\omega)dZ_t(\omega) \tag{5.65}$$

This integral belongs to a more general class of stochastic integrals, for which the underlying stochastic processes are the general Lévy processes. A rigorous construction is beyond this appendix and I only outline the procedures that are relevant to this chapter (see [16] for detailed information).

STEP 1: Define the integral for simple functions

$$\phi_n(t,\omega) = \sum_j \phi_{n,j}(\omega) \cdot \chi_{[t_j,t_{j+1})}(t) \tag{5.66}$$

where $\phi_{n,j}(\omega)$ is $\mathcal{F}_{t_j}$ measurable (Intuitively, this means the outcome is an observable.), and $\chi_{[t_j,t_{j+1})}(t)$ is the indicator function defined in (5.43). Then

$$\begin{aligned} \mathcal{I}[\phi_n](\omega) &= \int_0^T \phi_n(t,\omega)dZ_t(\omega) \\ &= \sum_j \phi_{n,j}(\omega)\left[Z_{t_{j+1}} - Z_{t_j}\right] \end{aligned} \tag{5.67}$$

STEP 2: If $\phi_n(t,\omega), \quad n \in \mathbb{N}$, converges to $f(t,\omega)$ in $L^2(P)$, i. e.

$$E\left[\int_0^T (f-\phi_n)^2 dt\right] \to 0 \qquad \text{as } n \to \infty \tag{5.68}$$

then

$$\mathcal{I}[f](\omega) = \lim_{n\to\infty} \int_0^T \phi_n(t,\omega)dZ_t(\omega) \tag{5.69}$$

Some useful properties of the Itô integral, which are applied in this chapter, are listed here:

$$\int_0^T f(t,\omega)dZ_t = \int_0^S f(t,\omega)dZ_t + \int_S^T f(t,\omega)dZ_t \qquad 0 \le S \le T \tag{5.70}$$

$$E\left[\int_0^T f(t,\omega)dZ_t\right] = 0 \tag{5.71}$$

$$E\left[\left(\int_0^T f(t,\omega)dZ_t\right)^2\right] = E\left[\int_0^T f^2(t,\omega)dt\right] \tag{5.72}$$

The last equation is also called the Itô isometry.

Itô Lemma

The Itô Lemma is a fundamental theorem to all the theoretical development of this chapter. It answers the question: if we know an Itô process X, what process does a function of X follow? I will only give the one dimensional Itô lemma:

Let X be an Itô process given by

$$dX_t = a(t,\omega)dt + b(t,\omega)dZ_t \tag{5.73}$$

Let $g(t,x) \in C^2([0,\infty) \times \mathbb{R})$. Then

$$Y_t = g(t, X_t)$$

is again an Itô process and satisfies

$$\begin{aligned} dY_t &= \left[\partial_t g(t,X_t) + a(t,\omega)\partial_x g(t,X_t) + \frac{1}{2}b^2(t,\omega)\partial_x^2 g(t,X_t)\right] dt \\ &\quad + b(t,\omega)\partial_x g(t,X_t)dZ_t \end{aligned} \tag{5.74}$$

The Itô lemma implies that we can use the following to manipulate the differentials:

$$dt \cdot dt = dt \cdot dZ_t = 0 \tag{5.75}$$

$$dZ_t \cdot dZ_t = dt \tag{5.76}$$

5.8.3 Martingales

A stochastic process M_t is a martingale with respect to a measure P if and only if

$$E^P[|M_t|] < \infty \qquad \text{for all } t \tag{5.77a}$$

$$E^P[M_s|\mathcal{F}_t] = M_t \qquad s \geq t \tag{5.77b}$$

where $\mathcal{F}_t$ is a sub σ-algebra belonging to a filtration. Without introducing detailed mathematical constructions, $\mathcal{F}_t$ has the meaning of a collection of all the information about the stochastic process M up to time t. A good example of a martingale is a Brownian motion: given that a Brownian particle starts from somewhere r_0 and now locates at r_t (these information is contained in $\mathcal{F}_t$), the expected location of this Brownian particle at some future time s is just its present location. This is very intuitive from the physics perspective and it is just what (5.77b) means.

A process X is a **sub-martingale** if

$$E^P[|X_t|] < \infty \qquad \text{for all } t \tag{5.78a}$$

$$E^P[X_s|\mathcal{F}_t] \geq X_t \qquad s \geq t \tag{5.78b}$$

and we call X a **super-martingale** if $-X$ is a sub-martingale.

Just like a cartesian coordinate system $(\hat{x}, \hat{y}, \hat{z})$ which spans a three dimensional space, the "space" of all martingales with respect to a measure P can be spanned by the standard Brownian motion Z under P.

Martingale Representation Theorem

Let Z be a standard Brownian motion with respect to a measure P. Suppose M is a martingale with respect to P, then there exists a unique stochastic process ϕ with $E[\int_0^t \phi_s^2 ds] < \infty$ such that

$$M_t(\omega) = E^P[M_0] + \int_0^t \phi(s, \omega) dZ_t \tag{5.79}$$

A direct consequence of the Martingale representation theorem to this chapter is that using Brownian motion to model a stochastic environment is complete (up to a drift term) except for the case when the environmental conditions can undergo a jump process. For this latter case a general Martingale representation for a Lévy process is needed.

5.8.4 Diffusion Properties

The solution of a stochastic differential equation can be thought of as a problem of a Brownian particle moving in a fluid, therefore, such stochastic processes are also called diffusions. A complete description of diffusion properties is not possible in this appendix so I will only introduce several of them which are relevant to this chapter.

Let X_t be an Itô diffusion process:

$$dX_t = a(X_t)dt + \sigma(X_t)dZ_t \tag{5.80}$$

The generator $\mathscr{G}$ of X_t is defined by

$$\mathscr{G}f(x) = \lim_{t\downarrow 0} \frac{E[f(X_t)|X_0 = x] - f(x)}{t} \tag{5.81}$$

The set of functions $f : \mathbb{R} \to \mathbb{R}$ which have the limit at x is denoted by $\mathcal{D}_{\mathscr{G}}(x)$. If $f \in C^2(\mathbb{R})$ then

$$\mathscr{G}f(x) = a(x)\partial_x f(x) + \frac{1}{2}\sigma^2(x)\partial_x^2 f(x) \tag{5.82}$$

Dynkin's Formula:

Let $f \in C^2(\mathbb{R})$. Then

$$E[f(X_t)|X_0 = x] = f(x) + E\left[\int_0^T \mathscr{G}f(X_t)dt \middle| X_0 = x\right] \tag{5.83}$$

Note that this formula is also true when T is a stopping time.

5.8.5 Jensen's Inequality

If $f : \mathbb{R} \to \mathbb{R}$ is a convex function and if X and $f(X)$ are both integrable, then

$$f(E(X)) \leq E[f(X)] \tag{5.84}$$

5.9 Appendix B: Dynamic Programming and the HJB Equation

This chapter applies extensively the technique of dynamical programming, so I include in this appendix some essential ingredients of the dynamical programming technique, from which I will give a derivation to the HJB equation (5.12). In short dynamic programming is a technique to solve problems which contain similar subproblems. In essence, dynamical programming is a searching algorithm which can reduce the complexity of searching from exponential to polynomial. To lay out the basic problem and algorithm, I will closely follow the book of *Bertsekas* [24]. For a more detailed description and proof, please refer to his book [Chapter 1 and Chapter 7]. The basic problem that is of interest to us is the following:

Suppose we are given a discrete-time dynamic system. The system is specified by a state variable x_k where k is an index for discrete time. The state variable involves in time according to

$$x_{k+1} = f_k(x_k, u_k, w_k) \ , \qquad k = 0, 1, \cdots, N-1 \tag{5.85}$$

u_k is a control that we can apply to the dynamic system and w_k is a noise or disturbance of which we only know its statistics. It is clear that our control u_k depends on our knowledge about the system at time k; in other words we have a mapping from x_k to u_k at every point in time

$$u_k = \mu_k(x_k) \tag{5.86}$$

We call a sequence of these mappings a policy:

$$\pi = \{\mu_0, \mu_1, \cdots, \mu_{N-1}\} \tag{5.87}$$

At each stage k there is a reward or cost (here I assume reward) function $g_k(x_k, u_k, w_k)$, $k = 0, 1, \cdots, N-1$ and $g_N(x_N)$. The expected reward given a feasible policy π is

$$J_\pi(x_0) = E\left[g_N(x_N) + \sum_{k=0}^{N-1} g_k(x_k, u_k, w_k)\right] \tag{5.88}$$

where the expectation is taken with respect to noise w_k. The objective is to find an optimal policy that maximizes $J_\pi(x_0)$:

$$J_{\pi^*}(x_0) = \max_\pi J_\pi(x_0) \tag{5.89}$$

The direct method to solve this problem is to enumerate all the possible ways of evolution and find out the one that maximizes the reward; however, this is computationally infeasible. The dynamic programming technique solve this problem in a backward fashion: We solve the last period maximization problem first, move one period backward, solve the $N-1$ period maximization problem and repeat this process until period 0. This technique is built on the principle of Optimality:

Principle of Optimality:

Let $\pi^* = \{\mu_0^*, \mu_1^*, \cdots, \mu_{N-1}^*\}$ be an optimal policy for the basic problem. Consider a sub problem where we are at period k to maximize the reward from time k on to period N:

$$E\left[g_N(x_N) + \sum_{j=k}^{N-1} g_j(x_j, u_j, w_j)\right] \tag{5.90}$$

The optimal policy $\{\mu_k^*, \mu_{k+1}^*, \cdots, \mu_{N-1}^*\}$ is optimal for this sub problem.

Based on this principle, the dynamic programming algorithm is given in the following:

Dynamic Programming Algorithm

The optimal reward $J^*(x_0)$ of the basic problem is equal to $J(x_0)$, which is obtained by the last step of the following algorithm which proceeds backward in time from period $N-1$ to period 0:

$$J_N(x_N) = g_N(x_N) \tag{5.91}$$

$$J_k(x_k) = \max_{u_k} \left\{ E\left[g_k(x_k, u_k, w_k) + J_{k+1}(f(x_k, u_k, w_k))\right]\right\}, \quad k = 0, 1, \cdots, N-1 \tag{5.92}$$

There are very few cases where the an analytic solution is available, so numerical methods are developed.

Suppose we are to solve the following problem: The dynamic system can exist in n states $1, 2, \cdots, n$. The reward function $g(u)$ is a $n-$vector function whose element $g_i(u)$ is the reward in state i, given control u. Let $P(x)$ be a transition probability matrix whose matrix element $P_{ij}(x)$ is the probability of transition from state i to state j given a control u is applied. The dynamic programming algorithm is to calculate

$$J_t = \max_u \left[g(u) + \lambda P(u) J_{t+1}\right] \tag{5.93}$$

where $\lambda \in (0, 1]$ is a parameter.

Backward Recursion

```
(1) Initialize $g(u)$, $P(u)$, $\lambda$, $J_N$ and $t \leftarrow N-1$;
(2) set $J_t \leftarrow \max_u [g(u) + \lambda P(u)J_{t+1}]$ and $u_t \leftarrow \operatorname{argmax}_u [g(u) + \lambda P(u)J_{t+1}]$;
(3) set $t \leftarrow t-1$;
(4) repeat the loop from (2) until $t = 0$.
```

For infinite horizon $N \to \infty$ problem, two numerical schemes can be used:

Function Iteration

```
(1) Initialize $g(u)$, $P(u)$, $\lambda$ and an initial guess for $J$;
(2) let $J \leftarrow \max_u [g(u) + \lambda P(u)J]$;
(3) repeat (2) until $\| \Delta J \| \leq$ tol;
(4) set $u \leftarrow \operatorname{argmax}_u [g(u) + \lambda P(u)J]$.
```

Policy Iteration

```
(1) Initialize $g(u)$, $P(u)$, $\lambda$ and an initial guess for $J$;
```

(2) let $u \leftarrow \underset{u}{\text{argmax}}\,[g(u) + \lambda P(u)J]$;

(3) let $J \leftarrow [I - \lambda P(u)]^{-1} g(u)$;

(4) repeat the iteration until $\| \Delta J \| \leq$ tol.

Now I derive (5.12) from the above discrete time dynamical programming technique. The value function is

$$J(N_t, \mathcal{I}_t, t) = \max_{\Phi_t} E_t[U(N_T)] \tag{5.94}$$

and the reward function is non-vanishing only for period T: $U(N_T)$. From (5.92) we have

$$J(N_t, \mathcal{I}_t, t) = \max_{\Phi_t} E_t[J(N_{t+\Delta t}, \mathcal{I}_{t+\Delta t}, t + \Delta t)] \tag{5.95}$$

Now apply Dynkin's formula (5.83) to the RHS of (5.95) to get

$$\begin{aligned} & E_t[J(N_{t+\Delta t}, \mathcal{I}_{t+\Delta t}, t + \Delta t)] \\ = \; & J(N_t, \mathcal{I}_t, t) + [\partial_t J + a(\Phi_t, N_t, \mathcal{I}_t)\partial_N J + \mu_I(\mathcal{I}_t)\partial_I J]\Delta t \\ + \; & \left[\frac{1}{2}(b^2(\Phi_t, N_t, \mathcal{I}_t)\partial_N^2 J + \sigma_I^2(\mathcal{I}_t)\partial_I^2 J) + \rho \; b(\Phi_t, N_t, \mathcal{I}_t)\sigma_I(\mathcal{I}_t)\partial_{N,I}^2 J\right] \Delta t \end{aligned} \tag{5.96}$$

where I have used the relations

$$N_{t+\Delta t} = N_t + a(\phi_t, N_t, \mathcal{I}_t)\Delta t + b(\phi_t, N_t, \mathcal{I}_t)\Delta Z_{E,t} + \mathcal{O}(\Delta t^2) \tag{5.97}$$

$$\mathcal{I}_{t+\Delta t} = \mathcal{I}_t + \mu_I(\mathcal{I}_t)\Delta t + \sigma_I(\mathcal{I}_t)\Delta Z_{I,t} + \mathcal{O}(\Delta t^2) \tag{5.98}$$

(5.3) and (5.76). Substituting (5.96) to (5.95) and rearrange terms I thus obtain

$$\begin{aligned} \max_{\Phi_t} \quad \{ \quad & \partial_t J + a(\Phi_t, N_t, \mathcal{I}_t)\partial_N J + \mu_I(\mathcal{I}_t)\partial_I J \\ + \quad & \frac{1}{2}[b^2(\Phi_t, N_t, \mathcal{I}_t)\partial_N^2 J + \sigma_I^2(\mathcal{I}_t)\partial_I^2 J] \\ + \quad & \rho \; b(\Phi_t, N_t, \mathcal{I}_t)\sigma_I(\mathcal{I}_t)\partial_{N,I}^2 J\}\Delta t = 0 \end{aligned} \tag{5.99}$$

(5.99) has to be true for arbitrary small but nonvanishing Δt so I obtain (5.12). The HJB equation can be proved with much more rigor and for general cases, please refer to [17].

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