Chapter 5
Conclusions and Discussion

In this chapter we shall conclude and discuss about the results and the methods obtained from the previous chapters.

5.1 Conclusions and Discussion

In this thesis, we have considered the problem of a single polymer chain in a quenched random medium with long-range interactions. The "quenched random medium" means the medium which has the fixed obstacles or scatterers distributed randomly. The main objective is to determine the size of the polymer chain. This polymer chain has long-range interaction with the obstacles. To solve this problem, first of all, we average the generalized Edwards' Hamiltonian over the random potential and consequently got the non-local term that included the correlation function. We assume that the interaction between an obstacle and a monomer along the polymer chain is the long-range interaction and in the Gaussian's form. It means that the correlation function is also the Gaussian. This correlation function represents the correlation among the monomers along the chain. It has been shown that at the beginning a flexible polymer embedded in quenched random medium has no correlation among the monomers but has the interaction with the obstacles only. After averaging the Hamiltonian over the random potential, this polymer behaves like the single polymer chain which has no obstacles but has the correlation between the monomers. The effects of this correlation depends on W_ξ, the magnitude of the fluctuation, as shown in

Eq. (4.15). ξ (the correlation length) is the farthest distance that still has the correlation. If the correlation length is short, the movement of any monomer will affect only the nearby monomers. However, if the correlation length is farther, the influence of the movement will be greater. Based on this model, the Feynman Path-Integral is, then, used to find out the solution. We begin by modeling the polymer Hamiltonian using a non-local quadratic trial Hamiltonian, Eq.(4.16), which can be calculated exactly. This translation invariant trial Hamiltonian is essential since it has the same symmetry as the averaged Hamiltonian, Eq.(4.15), which is translation invariance due to the random nature of the system. The calculation is proceeded by considering the differences between the polymer propagator, Eq.(4.17), and the trial propagator, Eq.(4.20), as the first cumulant approximation. The variational priciple, Eq.(4.40), is used to find the optimal values of the variational parameters. The size of the polymer chain can be determined. The results show that our caculation is well agree with the others. The limit can be considered in two ways, that is

Case I for the short-range correlation ($\xi \to 0$)

Our results are:

$$\left\langle \left(\vec{R}\,(N) - \vec{R}\,(0) \right)^2 \right\rangle_{\beta H_0(\omega)} \approx b^2 N \qquad , (\omega N \to 0) \tag{5.1}$$

and

$$\left\langle \left(\vec{R}\,(N) - \vec{R}\,(0) \right)^2 \right\rangle_{\beta H_0(\omega)} \approx \frac{b^2 u^4}{2} \left(\frac{3}{\pi^2 \xi^2 b^2} \right)^3 , (\omega N \to \infty) . \tag{5.2}$$

The results of Edwards and Muthukumar (1988) are:

$$\left\langle \overline{R^2} \right\rangle = N b^2, \left(\epsilon \mu^2 \rho_0^2 N b^6 \to 0 \right) \tag{5.3}$$

and

$$\left\langle \overline{R^2} \right\rangle = \frac{1}{\epsilon\mu^2\rho_0^2 b^4}, \left(\epsilon\mu^2\rho_0^2 N b^6 \to \infty\right). \tag{5.4}$$

Due to the definition the chain length L ($L = Nb$) is directly proportional to the number of segments N (or the total monomers) in the polymer chain. Therefore, we begin with considering in the case where the chain length is very short ($N \to 0$). According to Eq.(5.1), when $\omega N \to 0$ the polymer chain behaves like a free chain. This result is corresponding to the result of Edwards and Muthukumar (1988) in Eq.(5.3). On the contrary, if the polymer chain is very long ($N \to \infty$), as shown in Eq.(5.2), we can see that the size of a polymer chain is independent of the chain length. The polymer chain curls up in the free volume between the obstacles and the size of a polymer chain is limited by the size of the free volume. This result is corresponding to the result of Edwards and Muthukumar (1988) in Eq.(5.4).

Case II for the long-range correlation ($\xi \to \infty$)

Our results are:

$$\left\langle \left(\overrightarrow{R}(N) - \overrightarrow{R}(0)\right)^2 \right\rangle_{\beta H_0(\omega)} \approx b^2 N \qquad , (\omega N \to 0) \tag{5.5}$$

and

$$\left\langle \left(\overrightarrow{R}(N) - \overrightarrow{R}(0)\right)^2 \right\rangle_{\beta H_0(\omega)} \approx \frac{b^2 N}{4} \qquad , (\omega N \to \infty). \tag{5.6}$$

The result of Shiferaw and Goldschmidt (2000) is:

$$\overline{\left\langle \overrightarrow{R}^2 \right\rangle} = Nb^2 . (0 \leq N \leq \infty). \tag{5.7}$$

Eq.(5.5) and Eq.(5.6) show that the polymer chain always behaves like a free chain, these results are in good agreement with Shiferaw and Goldschmidt (2000) in Eq.(5.7). These results show that the polymer chain still behaves like

a free chain as if there is no random potential no matter how long the polymer chain is.

For the finite-correlation length we must solve the variational equation numerically. This method can be also generalized to include the excluded volume effect as discussed in Sa-Yakanit, Kunsombat and Niamploy (2000).