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Appendix A

A Non-Local Quadratic Propagator

In order to evaluate the averages, $\left\langle \overrightarrow{R}(\tau) \right\rangle_{\beta H_0(\omega)}$ and $\left\langle \overrightarrow{R}(\tau) \cdot \overrightarrow{R}(\sigma) \right\rangle_{\beta H_0(\omega)}$, it is nescessary to establish a characteristic functional as

$$\left\langle \exp\left(- \int_0^N d\tau \overrightarrow{f}(\tau) \cdot \overrightarrow{R}(\tau) \right) \right\rangle_{\beta H_0(\omega)}$$

$$= \frac{\int_0^N D\left[\overrightarrow{R}(\tau)\right] \exp\left(-\beta H_0(\omega) - \int_0^N d\tau \overrightarrow{f}(\tau) \cdot \overrightarrow{R}(\tau) \right)}{\int_0^N D\left[\overrightarrow{R}(\tau)\right] \exp(-\beta H_0(\omega))}, \qquad \text{(A.1)}$$

where $\overrightarrow{f}(\tau)$ is any arbitray function. Eq.(A.1) suggests that if the trial Hamiltonian $\beta H_0(\omega)$ is quadratic, then the Hamiltonian

$$\beta H_0^{'}(\omega) = \beta H_0(\omega) + \int_0^N d\tau \overrightarrow{f}(\tau) \cdot \overrightarrow{R}(\tau). \qquad \text{(A.2)}$$

From Feynman and Hibbs (1995), the path-integral of Eq.(A.1) can be carried out exactly as

$$\left\langle \exp\left(- \int_0^N d\tau \overrightarrow{f}(\tau) \cdot \overrightarrow{R}(\tau) \right) \right\rangle_{\beta H_0(\omega)} =$$

$$\exp\left(- \left[\beta H_{0,\min}^{'}\left(\overrightarrow{R}_2 - \overrightarrow{R}_1; N, \omega \right) - \beta H_{0,\min}\left(\overrightarrow{R}_2 - \overrightarrow{R}_1; N, \omega \right) \right] \right), \qquad \text{(A.3)}$$

where $\beta H_{0,\min}^{'}\left(\overrightarrow{R}_2 - \overrightarrow{R}_1; N, \omega \right)$ and $\beta H_{0,\min}\left(\overrightarrow{R}_2 - \overrightarrow{R}_1; N, \omega \right)$ are the corresponding minimum Hamiltonians of $\beta H_0^{'}(\omega)$ and $\beta H_0(\omega)$ respectively. These minimum Hamiltonians can be obtained from the most probable chain configuration method (Wiegel, 1986) by minimization of the Hamiltonian. To do this we make a variation on $\beta H_0^{'}(\omega)$ in Eq.(A.2) and thus obtain an equation

$$\frac{d^2\vec{R}_c(\tau)}{d\tau^2} - \frac{\omega^2}{N}\int_0^N d\sigma\left(\vec{R}_c(\tau) - \vec{R}_c(\sigma)\right) = \frac{b^2\vec{f}(\tau)}{3}. \tag{A.4}$$

This equation may be rewritten in the form

$$\frac{d^2\vec{R}_c(\tau)}{d\tau^2} - \omega^2\vec{R}_c(\tau) = -\frac{\omega^2}{N}\int_0^N d\sigma\vec{R}_c(\sigma) + \frac{b^2\vec{f}(\tau)}{3} \tag{A.5}$$

and introducing a Green Function

$$\left(\frac{d^2}{d\tau^2} - \omega^2\right)g(\tau,\sigma) = \delta(\tau,\sigma), \tag{A.6}$$

where

$$g(\tau,\sigma) = -\frac{\sinh\omega(N-\tau)\sinh\omega\sigma\Theta(\tau-\sigma)}{\omega\sinh\omega N} - \frac{\sinh\omega(N-\sigma)\sinh\omega\tau\Theta(\sigma-\tau)}{\omega\sinh\omega N} \tag{A.7}$$

with Θ denoting the Heviside step function, then the general solution of Eq.(A.6) with the boundary condition $\vec{R}(0) = \vec{R}_1$ and $\vec{R}(N) = \vec{R}_2$ can be written as

$$\vec{R}_c(\tau) = \frac{\left[\vec{R}_2\sinh\omega\tau + \vec{R}_1\sinh\omega(N-\tau)\right]}{\sinh\omega N} + \int_0^N\left[\frac{b^2\vec{f}(\sigma)}{3} - \frac{\omega^2}{N}\int_0^N d\sigma\vec{R}(\sigma)\right]g(\tau,\sigma)\,d\sigma. \tag{A.8}$$

This Eq.(A.8) is an integral equation which can be solved and the solution is

$$\vec{R}_c(\tau) = \frac{\left[\vec{R}_2\sinh\omega\tau + \vec{R}_1\sinh\omega(N-\tau)\right]}{\sinh\omega N} + \int_0^N\frac{b^2\vec{f}(\sigma)}{3}g(\tau,\sigma)\,d\sigma + \frac{\left(\vec{R}_1+\vec{R}_2\right)\sinh\frac{\omega\tau}{2}\sinh\frac{\omega(N-\tau)}{2}}{\cosh\frac{\omega N}{2}} - \frac{4b^2\sinh\frac{\omega\tau}{2}\sinh\frac{\omega(N-\tau)}{2}\int_0^N\vec{f}(\sigma)\sinh\frac{\omega\sigma}{2}\sinh\frac{\omega(N-\sigma)}{2}}{3\omega\sinh\omega N}. \tag{A.9}$$

The minimum Hamiltonian $\beta H'_{0,\min}\left(\overrightarrow{R}_2-\overrightarrow{R}_1;N,\omega\right)$ is simply obtained by substituting $\overrightarrow{R}_c$ from Eq.(A.9) into the expression below

$$\beta H'_{0,\min}\left(\overrightarrow{R}_2-\overrightarrow{R}_1;N,\omega\right)=\frac{3}{2b^2}\int_0^N d\tau\dot{\overrightarrow{R}}_c^2(\tau)$$
$$+\frac{3\omega^2}{4Nb^2}\int_0^N\int_0^N d\tau d\sigma\left[\overrightarrow{R}_c(\tau)-\overrightarrow{R}_c(\sigma)\right]^2+\int_0^N d\tau\overrightarrow{f}(\tau)\cdot\overrightarrow{R}_c(\tau)$$
$$=\frac{3}{2b^2}\left[\dot{\overrightarrow{R}}_c(N)\cdot\overrightarrow{R}_c(N)-\dot{\overrightarrow{R}}_c(0)\cdot\overrightarrow{R}_c(0)\right].\qquad\text{(A.10)}$$

This give

$$\beta H'_{0,\min}\left(\overrightarrow{R}_2-\overrightarrow{R}_1;N,\omega\right)=\frac{3\omega}{4b^2}\coth\frac{\omega N}{2}\left[\overrightarrow{R}_2-\overrightarrow{R}_1\right]^2+\frac{3\omega}{2b^2\sinh\omega N}$$
$$\times[\frac{2b^2\overrightarrow{R}_2}{3\omega}\int_0^N d\tau\overrightarrow{f}(\tau)\left(\sinh\frac{\omega\tau}{2}+2\sinh\frac{\omega N}{2}\sinh\frac{\omega\tau}{2}\sinh\frac{\omega(N-\tau)}{2}\right)$$
$$+\frac{2b^2\overrightarrow{R}_1}{3\omega}\int_0^N d\tau\overrightarrow{f}(\tau)\left(\sinh\frac{\omega(N-\tau)}{2}+2\sinh\frac{\omega N}{2}\sinh\frac{\omega\tau}{2}\sinh\frac{\omega(N-\tau)}{2}\right)$$
$$-\frac{2b^4}{3^2\omega^2}\int_0^N\int_0^\tau d\tau d\sigma\overrightarrow{f}(\tau)\cdot\overrightarrow{f}(\sigma)\left(\sinh\omega(N-\tau)\sinh\omega\sigma\right.$$
$$\left.+4\sinh\frac{\omega\tau}{2}\sinh\frac{\omega(N-\tau)}{2}\sinh\frac{\omega\sigma}{2}\sinh\frac{\omega(N-\sigma)}{2})\right]\}.\qquad\text{(A.11)}$$

The minimum Hamiltonian $\beta H_{0,\min}\left(\overrightarrow{R}_2-\overrightarrow{R}_1;N,\omega\right)$ is then obtained by setting $\overrightarrow{f}(\tau)=0$ in Eq.(A.11).

$$\beta H_{0,\min}\left(\overrightarrow{R}_2-\overrightarrow{R}_1;N,\omega\right)=\frac{3\omega}{4b^2}\coth\frac{\omega N}{2}\left[\overrightarrow{R}_2-\overrightarrow{R}_1\right]^2\qquad\text{(A.12)}$$

Next, let us evaluate the trial propagator $\overline{G}_0\left(\overrightarrow{R}_2,\overrightarrow{R}_1;N,\omega\right)$ in Eq.(4.18). We can rewrite the trial Hamiltonian $\beta H_0(\omega)$ in Eq.(4.16) in the form

$$\beta H_0(\omega)=\beta H_{Ho}-\frac{3\omega^2}{2Nb^2}\left[\int_0^N d\tau\overrightarrow{R}(\tau)\right]^2,\qquad\text{(A.13)}$$

where βH_{Ho} is the harmonic oscillator Hamiltonian

$$\beta H_{Ho}=\frac{3}{2b^2}\int_0^N d\tau\left(\dot{\overrightarrow{R}}^2(\tau)+\omega^2\overrightarrow{R}^2(\tau)\right).\qquad\text{(A.14)}$$

The exponential of the second term of Eq.(A.13) can be converted to an integral form by an identity

$$\exp\left(\frac{3\omega^2}{2Nb^2}\left[\int_0^N d\tau \vec{R}(\tau)\right]^2\right) = \left(\frac{Nb^2}{6\pi\omega^2}\right)^{3/2}\int d\vec{f}$$

$$\times \exp\left(-\frac{Nb^2\vec{f}^2}{6\omega^2} - \int_0^N d\tau \vec{R}(\tau)\cdot\vec{f}\right). \qquad \text{(A.15)}$$

From Eq.(A.13) and Eq.(A.15) we find that the trial propagator $\overline{G}_0\left(\vec{R}_2, \vec{R}_1; N, \omega\right)$ can be expressed as

$$\overline{G}_0\left(\vec{R}_2, \vec{R}_1; N, \omega\right) = \left(\frac{Nb^2}{6\pi\omega^2}\right)^{3/2}\int_{\vec{R}_1}^{\vec{R}_2} D\left[\vec{R}(\tau)\right]\int d\vec{f}$$

$$\times \exp\left(-\beta H_{Ho} - \frac{Nb^2\vec{f}^2}{6\omega^2} - \int_0^N d\tau \vec{R}(\tau)\cdot\vec{f}\right). \qquad \text{(A.16)}$$

Changing the order of integration, Eq.(A.16) becomes

$$\overline{G}_0\left(\vec{R}_2, \vec{R}_1; N, \omega\right) = \left(\frac{Nb^2}{6\pi\omega^2}\right)^{3/2}\int d\vec{f}$$

$$\times \exp\left(-\frac{Nb^2\vec{f}^2}{6\omega^2}\right) G_{\vec{f}}\left(\vec{R}_2, \vec{R}_1; N, \vec{f}\right), \qquad \text{(A.17)}$$

where

$$G_{\vec{f}}\left(\vec{R}_2, \vec{R}_1; N, \vec{f}\right) = \int_{\vec{R}_1}^{\vec{R}_2} D\left[\vec{R}(\tau)\right]$$

$$\times \exp\left(-\beta H_{Ho} - \int_0^N d\tau \vec{R}(\tau)\cdot\vec{f}\right). \qquad \text{(A.18)}$$

The propagator Eq.(A.18) is the forced harmonic oscillator propagator with a constant external force $\vec{f}$, which is

$$G_{\vec{f}}\left(\vec{R}_2, \vec{R}_1; N, \vec{f}\right) = \left(\frac{3\omega^2}{2\pi b^2 \sinh \omega N}\right)^{3/2}$$

$$\times \exp[-(\frac{3\omega}{4b^2}\left(\coth\frac{\omega N}{2}\left[\vec{R}_2 - \vec{R}_1\right]^2 + \tanh\frac{\omega N}{2}\left(\vec{R}_2 + \vec{R}_1\right)^2\right)$$

$$+\frac{1}{\omega}\tanh\frac{\omega N}{2}\left(\vec{R}_2+\vec{R}_1\right)\cdot\vec{f}+\left(\frac{b^2}{3\omega^3}\tanh\frac{\omega N}{2}-\frac{Nb^2\vec{f}^2}{6\omega^2}\right))]. \tag{A.19}$$

Substituting Eq.(A.19) into Eq.(A.17), and performing the $\vec{f}$ - integration ,we get

$$\overline{G}_0\left(\vec{R}_2,\vec{R}_1;N,\omega\right)=\left(\frac{3}{2\pi Nb^2}\right)^{3/2}\left(\frac{\omega N}{2\sinh\frac{\omega N}{2}}\right)^3$$
$$\times\exp\left\{-\frac{3\omega}{4b^2}\coth\frac{\omega N}{2}\left|\vec{R}_2-\vec{R}_1\right|^2\right\}. \tag{A.20}$$

Vitae

Mr.Cherdsak Kunsombat was born on May 19, 1967 in Kanchanaburi. He received a B.Sc. degree in Physics from Kasetsart University in 1990 and a M.S. degree in Physics from Chulalongkorn University in 1993. He has been an instructor at Kasetsart University since 1994.