

# Monte Carlo methods and Dissipative Environments

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# Dissipative environments

## Path Integral

$$Z = \int e^{-S[q, x_\alpha]} \mathcal{D}[q, x_\alpha]$$

## Caldeira Legget Model

$$S[q, x_\alpha] = S_{\text{System}}[q] + S_{\text{Env}}[x_\alpha] + q \sum_{\alpha} c_{\alpha} x_{\alpha}$$

$$S_{\text{Env}} = \int \sum_{\alpha} \{ m_{\alpha} \dot{x}_{\alpha}^2 + m_{\alpha} \omega_{\alpha}^2 x_{\alpha} \}$$

$$S_{\text{System}} = \int_{\tau} M \dot{q}_{\tau}^2$$

Integrating over the Environment Degrees of freedom

$$S_{\text{Dissipation}} = \eta \iint \frac{\pi^2 T^2 (q_{\tau} - q_{\tau'})^2}{\sin^2 \pi T (\tau - \tau')} d\tau d\tau'$$

For large  $T$   $S_{\text{Dissipation}} = \int_{\tau} \eta \dot{q}_{\tau}$

## Model

Particle on a Ring ( $R = 1$ )

$$S[\theta] = \int_{\tau} M \dot{\theta}_{\tau}^2 + \eta \iint \frac{\pi^2 T^2 \sin^2 (\theta_{\tau} - \theta_{\tau'})}{\sin^2 \pi T (\tau - \tau')} d\tau d\tau'$$

Magnetic flux  $\phi_x$

$$Z = \sum_{m=-\infty}^{\infty} e^{2\pi i m \phi_x} \int_{\mathcal{D}[\theta]} e^{-S[\theta^{(m)}]}$$

Interest in the velocity correlation function

$$K(\tau) = \left\langle \dot{\theta}_t \dot{\theta}_{t-\tau} \right\rangle = \frac{\sum_m e^{2\pi i m \phi_x} \int_{\mathcal{D}[\theta]} \dot{\theta}_t \dot{\theta}_{t-\tau} e^{-S[\theta^{(m)}]}}{\sum_m e^{2\pi i m \phi_x} \int_{\mathcal{D}[\theta]} e^{-S[\theta^{(m)}]}}$$

$$K(\omega) = T\omega^2 \langle |\theta_{\omega}|^2 \rangle = K_0 + K_1 |\omega| + \mathcal{O}(\omega^2)$$

$K_1$  the dissipation term

## Path Integral Monte Carlo

Minimization of the action by Markov Chain



### Detail Balance

$$\pi(a)p(a \rightarrow b) = \pi(b)p(b \rightarrow a)$$

$\pi(a)$  stationary probability to be in state  $a$

$p(a \rightarrow b)$  transition probability states  $a$  and  $b$

Metropolis algorithm, any step is accepted with

$$p(a \rightarrow b) = \begin{cases} 1 & \pi(b) > \pi(a) \\ \pi(b)/\pi(a) & \pi(b) < \pi(a) \end{cases}$$

## Back to the Model

### Stationary Probability

$$\pi(\theta) = \sum_m e^{2\pi i m \phi_x} e^{-S[\theta^{(m)}]}$$

### Markov Chain

$$\theta_\tau \rightarrow \theta_\tau \pm A \quad ; \quad \theta_\omega \rightarrow \theta_\omega \pm A_\omega$$

### Numerical Results for the velocity correlation

