2. Dynamic perturbation theory and renormalization group

2.1. Response functional

general Langevin equation: $\frac{\partial S^\alpha(\vec{x},t)}{\partial t} = \underbrace{F^\alpha[\vec{S}](\vec{x},t)} + \zeta^\alpha(\vec{x},t)$

$= F^\alpha_{rev} + F^\alpha_{rel}, \quad F^\alpha_{rel} = -D^\alpha (i\vec{\nabla})^{a_\alpha} \frac{\delta H}{\delta S^\alpha}$

$\langle \zeta^\alpha(\vec{x},t)\rangle = 0, \quad \langle \zeta^\alpha(\vec{x},t)\zeta^\beta(\vec{x}',t')\rangle = 2\underbrace{L^\alpha}\, \delta(\vec{x}-\vec{x}')\,\delta(t-t')\,\delta^{\alpha\beta}$

can be operator, e.g. $\sim D^\alpha \vec{\nabla}^2$ for conserved field

associated noise probability distribution: assumed Gaussian

$$W[\vec{\zeta}] \sim \exp\left(-\frac{1}{4}\int d^dx \int dt \sum_\alpha \zeta^\alpha(\vec{x},t)\left[\underbrace{(L^\alpha)^{-1}} \zeta^\alpha(\vec{x},t)\right]\right)$$

inverse operator (Green's function)

change variables to mesoscopic fields via $\zeta^\alpha = \frac{\partial S^\alpha}{\partial t} - F^\alpha[\vec{S}]$

$\rightarrow W[\vec{\zeta}]\,\mathcal{D}[\vec{\zeta}] = P[\vec{S}]\,\mathcal{D}[\vec{S}] \sim e^{-G[\vec{S}]}\,\mathcal{D}[\vec{S}]$ with statistical weight given by Onsager-Machlup functional:

$$G[\vec{S}] = \frac{1}{4}\int d^dx \int dt \sum_\alpha \left(\frac{\partial S^\alpha(\vec{x},t)}{\partial t} - F^\alpha[\vec{S}](\vec{x},t)\right)\left[(L^\alpha)^{-1}\left(\frac{\partial S^\alpha(\vec{x},t)}{\partial t} - F^\alpha[\vec{S}](\vec{x},t)\right)\right]$$

note: Jacobian for variable transformation depends on discretization:

$t_l = t_0 + l\tau, \quad S^\alpha_l = S^\alpha(t_l), \quad F^\alpha_l = F^\alpha[\vec{S}](t_l)$:

$\frac{1}{\tau}(S^\alpha_{l+1} - S^\alpha_l) = \kappa F^\alpha_{l+1} + (1-\kappa)F^\alpha_l + \zeta^\alpha_l, \quad 0 \leq \kappa \leq 1$

$\rightarrow \underbrace{\frac{\partial \zeta^\alpha_l}{\partial S^\alpha_{l+1}} = \frac{1}{\tau} - \kappa \frac{\partial F^\alpha_{l+1}}{\partial S^\alpha_{l+1}}}_{\text{diagonal}}, \quad \underbrace{\frac{\partial \zeta^\alpha_l}{\partial S^\alpha_l} = -\frac{1}{\tau} - (1-\kappa)\frac{\partial F^\alpha_l}{\partial S^\alpha_l}}_{\text{subdiagonal}}$ in Jacobian matrix

$\rightarrow$ determinant $\sim \prod_l \frac{1}{\tau}\left(1 - \kappa\tau \frac{\partial F^\alpha_{l+1}}{\partial S^\alpha_{l+1}}\right) \sim e^{-\kappa \sum_l \tau \frac{\partial F^\alpha_{l+1}}{\partial S^\alpha_{l+1}}}$

yields additional term in Onsager-Machlup functional

$$\kappa \int d^dx \int dt \sum_\alpha \frac{\delta F^\alpha[\vec{S}]}{\delta S^\alpha(\vec{x},t)}$$

not present for forward discretization in time: $\kappa = 0$

Itô calculus for stochastic differential equations inconvenient for computations: inverse operator L^{-1}, high non-linearities $\sim (F^\alpha)^2$

linearize by means of Gaussian integral over auxiliary "response" fields $\tilde{S}^\alpha$

desired functional integral weight over noise histories:

$$\langle A[\vec{\zeta}]\rangle_\zeta \sim \int \mathcal{D}[\vec{\zeta}]\, A[\vec{S}[\vec{\zeta}]]\, W[\vec{\zeta}]$$

change variables $\vec{\zeta} \to \vec{S}$, impose constraint on Langevin dynamics:

$$1 = \int \mathcal{D}[\vec{S}] \prod_\alpha \prod_{(\vec{x},t)} \delta\left(\frac{\partial S^\alpha}{\partial t} - F^\alpha[\vec{S}] - \zeta^\alpha\right)$$

discretized in space-time, forward time discretization

$$\to \int \mathcal{D}[i\vec{\tilde{S}}] \int \mathcal{D}[\vec{S}] \exp\left[-\int d^dx \int dt \sum_\alpha \tilde{S}^\alpha \left(\frac{\partial S^\alpha}{\partial t} - F^\alpha[\vec{S}] - \zeta^\alpha\right)\right]$$

Fourier representation of Dirac delta

back to continuum limit

$$\to \langle A[\vec{S}]\rangle_\zeta \sim \int \mathcal{D}[i\vec{\tilde{S}}] \int \mathcal{D}[\vec{S}]\, A[\vec{S}]\, e^{-\int d^dx \int dt \sum_\alpha \tilde{S}^\alpha \left(\frac{\partial S^\alpha}{\partial t} - F^\alpha[\vec{S}]\right)}.$$

noise average: $\cdot \int \mathcal{D}[\vec{\zeta}]\, e^{-\int d^dx \int dt \sum_\alpha \left[\frac{1}{4}\zeta^\alpha (L^\alpha)^{-1}\zeta^\alpha - \tilde{S}^\alpha \zeta^\alpha\right]}$

$$\sim e^{\int d^dx \int dt \sum_\alpha \tilde{S}^\alpha L^\alpha \tilde{S}^\alpha}$$

Gaussian integral, completing square:

$$\zeta^\alpha \to \tilde{\zeta}^\alpha = \zeta^\alpha - 2L^\alpha \tilde{S}^\alpha$$

so $P[\vec{S}] \sim \int \mathcal{D}[i\vec{\tilde{S}}]\, e^{-A[\vec{\tilde{S}},\vec{S}]}$

with <u>Janssen-De Dominicis response functional</u>

$$A[\vec{\tilde{S}},\vec{S}] = \int d^dx \int dt \sum_\alpha \left[\tilde{S}^\alpha(\vec{x},t)\underbrace{\left(\frac{\partial S^\alpha(\vec{x},t)}{\partial t} - F^\alpha[\vec{S}](\vec{x},t)\right)}_{\text{deterministic Langevin terms}} - \underbrace{\tilde{S}^\alpha(\vec{x},t) L^\alpha \tilde{S}^\alpha(\vec{x},t)}_{\text{noise correlator}}\right]$$

encodes:

note: integrate out auxiliary fields $\tilde{S}^\alpha \to$ Onsager-Machlup functional

e.g., for relaxational models A/B: $A = A_0 + A_{int}$,

linear, Gaussian part:

$$A_0[\vec{\tilde{S}},\vec{S}] = \int d^dx \int dt \sum_\alpha \left(\tilde{S}^\alpha(\vec{x},t)\left[\frac{\partial}{\partial t} + D(i\vec{\nabla})^a (r - \vec{\nabla}^2)\right] S^\alpha(\vec{x},t) - D\tilde{S}^\alpha(\vec{x},t)(i\vec{\nabla})^a\left[h^\alpha(\vec{x},t) + k_BT\tilde{S}^\alpha(\vec{x},t)\right]\right)$$

non linear, interaction:

$$A_{int}[\vec{\tilde{S}},\vec{S}] = D\frac{u}{6}\int d^dx \int dt \sum_{\alpha,\beta} \tilde{S}^\alpha(\vec{x},t)(i\vec{\nabla})^a S^\alpha(\vec{x},t)\, S^\beta(\vec{x},t)^2$$

→ dynamic susceptibility: (for $a=2$: integration by parts twice)

$$\chi^{\alpha\beta}(\vec{x}-\vec{x}', t-t') = \frac{\delta\langle S^\alpha(\vec{x},t)\rangle}{\delta h^\beta(\vec{x}',t')} = D\langle S^\alpha(\vec{x},t)(i\vec{\nabla})^a \tilde{S}^\beta(\vec{x}',t')\rangle$$

→ $\tilde{S}^\alpha$: "response fields"

1.2. Jarzynski's work theorem, Crooks' relation, fluctuation-dissipation theorem

scenario: $t \leq 0$ system Hamiltonian H_0, equilibrium at temperature T

$t > 0$: external field $\vec{h}(\vec{x},t)$ drives non-equilibrium dynamics

$t \geq t_f$: $\vec{h}$ fixed, new Hamiltonian H_1, relaxation to new equilibrium

also: time-reversed protocol: $\hat{\vec{h}}(\vec{x},t) = \vec{h}(\vec{x}, t_f - t)$

$O(n)$ LGW model: explicit time dependence $\dfrac{\partial H[\vec{S}](t)}{\partial t} = -\int d^dx \sum_\alpha S^\alpha(\vec{x}) \dfrac{\partial h^\alpha(\vec{x},t)}{\partial t}$

→ observable average: $\langle A[\vec{S}]\rangle = \int \mathcal{D}[\vec{S}_0] \dfrac{1}{Z_0(T)} e^{-H_0[\vec{S}]/k_BT}$ (equilibrium canonical ensemble, $t<0$)

$$\int \mathcal{D}[\vec{S}_1] \int \mathcal{D}[i\tilde{\vec{S}}] \int_{\vec{S}(\vec{x},0)=\vec{S}_0}^{\vec{S}(\vec{x},t_f)=\vec{S}_1} \mathcal{D}[\vec{S}]\, A[\vec{S}]\, e^{-\mathcal{A}[\tilde{\vec{S}},\vec{S}]}$$

$$\mathcal{A}[\tilde{\vec{S}},\vec{S}] = \int d^dx \int_0^{t_f} dt \sum_\alpha \tilde{S}^\alpha(\vec{x},t)\left[\frac{\partial S^\alpha(\vec{x},t)}{\partial t} + D(i\vec{\nabla})^a \frac{\delta H[\vec{S}](t)}{\delta S^\alpha(\vec{x},t)} - Dk_BT(i\vec{\nabla})^a \tilde{S}^\alpha(\vec{x},t)\right]$$

<u>variable transformation</u>: $\bar{S}^\alpha(\vec{x},t) = -\tilde{S}^\alpha(\vec{x},t) + \dfrac{1}{k_BT}\dfrac{\delta H[\vec{S}]}{\delta S^\alpha(\vec{x},t)}$

$$\Rightarrow \mathcal{A}[\tilde{\vec{S}},\vec{S}] = \int d^dx \int_0^{t_f} dt \sum_\alpha \Bigg(\bar{S}^\alpha(\vec{x},t)\left[\frac{\partial S^\alpha(\vec{x},t)}{\partial(-t)} + D(i\vec{\nabla})^a \frac{\delta H[\vec{S}](t)}{\delta S^\alpha(\vec{x},t)} - Dk_BT(i\vec{\nabla})^a \bar{S}^\alpha(\vec{x},t)\right]$$

$$+ \underbrace{\frac{1}{k_BT}\frac{\delta H[\vec{S}]}{\delta S^\alpha(\vec{x},t)}\frac{\partial S^\alpha(\vec{x},t)}{\partial t}\Bigg)}$$

$$= \int_0^{t_f} dt\left[\frac{dH[\vec{S}](t)}{dt} - \frac{\partial H[\vec{S}](t)}{\partial t}\right] = H_1[\vec{S}_1] - H_0[\vec{S}_0] - W_J[\vec{S}]$$

with Jarzynski's non-equilibrium work: $W_J[\vec{S}] = \displaystyle\int_0^{t_f} \frac{\partial H[\vec{S}](t)}{\partial t}\, dt$

note: in the absence of drive: these terms all vanish,

→ <u>equilibrium symmetry transformation</u> under time inversion

$\hat{A}[\vec{S}(\vec{x},t)] = A[\vec{S}(\vec{x},t_f - t)]$ for time-reversed protocol "R"

$$\langle A[\vec{S}]\rangle = \frac{Z_1(T)}{Z_0(T)} \int \mathcal{D}[\vec{S}_0] \int_{\vec{S}(\vec{x},0)=\vec{S}_0} \mathcal{D}[\vec{S}_1] \frac{1}{Z_1(T)} e^{-H_1[\vec{S}_1]/k_BT}$$ (equilibrium ensemble, $t > t_f$)

$$\int \mathcal{D}[i\tilde{\vec{S}}] \int_{\vec{S}(\vec{x},t_f)=\vec{S}_1} \mathcal{D}[\vec{S}]\, \hat{A}[\vec{S}]\, e^{\hat{W}_\gamma[\vec{S}]/k_BT - \mathcal{A}[\tilde{\vec{S}},\vec{S}]}$$

free energy difference $\Delta F = F_1 - F_0 = k_BT \ln \frac{Z_0(T)}{Z_1(T)}$

W_γ odd under time reversal: $\langle A[\vec{S}]\rangle = e^{-\Delta F/k_BT} \langle \hat{A}[\vec{S}] e^{-W_\gamma[\vec{S}]/k_BT}\rangle_R$

or $A'[\vec{S}] = A[\vec{S}]\, e^{-W_\gamma[\vec{S}]/k_BT}$:

$$\langle A[\vec{S}]\, e^{-W_\gamma[\vec{S}]/k_BT}\rangle = e^{-\Delta F/k_BT} \langle \hat{A}[\vec{S}]\rangle_R$$

$A = 1 \rightarrow$ Jarzynski's identity, work theorem: $\langle e^{-W_\gamma[\vec{S}]/k_BT}\rangle = e^{-\frac{\Delta F}{k_BT}}$

since $e^{-x} \geq 1 - x$: $\Delta F = -k_BT \ln \langle e^{-W_\gamma[\vec{S}]/k_BT}\rangle \leq \langle W_\gamma[\vec{S}]\rangle$

corollary of second law of thermodynamics

$$A[\vec{S}] = e^{-\lambda W_\gamma[\vec{S}]} \rightarrow \langle e^{-\lambda W_\gamma[\vec{S}]}\rangle = e^{-\Delta F/k_BT} \langle e^{\lambda W_\gamma[\vec{S}]} e^{-W_\gamma[\vec{S}]/k_BT}\rangle_R$$

$\rightarrow$ characteristic function for work probability distribution: $\beta = \frac{1}{k_BT}$

$$\chi(\lambda) = \int P(W_\gamma)\, e^{-\lambda W_\gamma}\, dW_\gamma = \langle e^{-\lambda W_\gamma}\rangle = e^{-\beta\Delta F} \chi(\beta - \lambda)_R$$

Laplace transform $\rightarrow$ Crooks' relation $\frac{P(W_\gamma)}{P_R(-W_\gamma)} = e^{(W_\gamma - \Delta F)/k_BT}$

$$\frac{\delta W_\gamma[\vec{S}]}{\delta h^\beta(\vec{x}',t')} = \frac{\partial S^\beta(\vec{x}',t')}{\partial t'}$$ (integrate by parts)

$$\rightarrow \frac{\delta}{\delta h^\beta(\vec{x}',t')} \langle A[\vec{S}]\, e^{-W_\gamma[\vec{S}]/k_BT}\rangle - e^{-\Delta F/k_BT} \frac{\delta \langle \hat{A}[\vec{S}]\rangle_R}{\delta h^\beta(\vec{x}',t')} =$$

only acts on A (fixed protocol, W_γ)

$$= \frac{1}{k_BT} \langle A[\vec{S}] \frac{\partial S^\beta(\vec{x}',t')}{\partial t'} e^{-W_\gamma[\vec{S}]/k_BT}\rangle$$

non-equilibrium fluctuation theorem

(usefulness really unclear...)

thermal equilibrium: $\Delta F = 0 = W_\gamma[\vec{S}]$, let $A[\vec{S}] = S^\alpha(\vec{x},t)$:

$$\frac{\delta \langle S^\alpha(\vec{x},t)\rangle}{\delta h^\beta(\vec{x}',t')} - \underbrace{\frac{\delta \langle S^\alpha(\vec{x},t_f - t)\rangle}{\delta h^\beta(\vec{x}',t_f - t')}}_{=0 \text{ causality}} = \frac{1}{k_BT} \frac{\partial}{\partial t'} \langle S^\alpha(\vec{x},t)\, S^\beta(\vec{x}',t')\rangle$$

$t > t'$: fluctuation-dissipation theorem

$$\rightarrow \chi^{\alpha\beta}(\vec{x}-\vec{x}', t-t') = \frac{\Theta(t-t')}{k_BT} \frac{\partial}{\partial t'} \langle S^\alpha(\vec{x},t)\, S^\beta(\vec{x}',t')\rangle = -\frac{\Theta(t-t')}{k_BT} \frac{\partial}{\partial t} \langle S^\alpha(\vec{x},t)\, S^\beta(\vec{x}',t')\rangle$$