Fourier Monte Carlo Renormalization Group Approach to Crystalline Membranes

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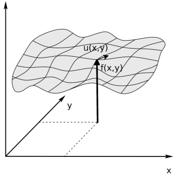
Flat Phase Effective Hamiltonian for Crystalline Membrane

Monge parametrization of deformations of a “flat” crystalline membrane w.r.t. suitable reference plane with coordinates $\boldsymbol{x} = (x, y)$:

- in-plane and out-of-plane deformations $\boldsymbol{u}(x, y),\ f(x, y)$
- Lagrangian strain tensor: drop nonlinear terms in u_i but keep $\partial_i f \partial_j f$ of f:



$$\epsilon_{ij} = \frac{1}{2}\left(g_{ij} - \delta_{ij}\right) \approx \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} + \frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j}\right)$$

- effective Hamiltonian $\mathcal{H}[f, \boldsymbol{u}] = \mathcal{H}^b[f] + \mathcal{H}^s[f, \boldsymbol{u}]$ is sum of out-of-plane bending and in-plane stretching energy

$$\mathcal{H}^b_\Lambda[f] = \frac{\kappa}{2}\int d^2x\,(\Delta f)^2\,, \qquad \mathcal{H}^s[f, \boldsymbol{u}] = \frac{1}{2}\sum_{ij}\int d^2x\left(2\mu\epsilon_{ij}^2 + \lambda\epsilon_{ii}\epsilon_{jj}\right)$$

- in-plane deformations u_i enter only harmonically: Gaussian integration yields effective Hamiltonian reflecting effective long range interaction for out-of-plane deformations f (with 2d Young's modulus $K = 4\mu(\mu+\lambda)/(2\mu+\lambda)$)

$$\boxed{\mathcal{H}[f] = \frac{\kappa}{2}\int\frac{d^2q}{(2\pi)^2}q^4|\tilde{f}(\boldsymbol{q})|^2 + \frac{K}{2}\int\frac{d^2Q}{(2\pi)^2}|\tilde{\mathcal{F}}(\boldsymbol{Q})|^2}, \qquad \boxed{\tilde{\mathcal{F}}(\boldsymbol{Q}) = \int\frac{d^2q}{(2\pi)^2}\left(\frac{\boldsymbol{Q}}{|\boldsymbol{Q}|}\times\boldsymbol{q}\right)\tilde{f}(\boldsymbol{q})\tilde{f}(\boldsymbol{Q}-\boldsymbol{q})}$$

- displacement correlations and mean-squared displacement governed by single exponent η:

$$\tilde{G}(\boldsymbol{q}) = \langle\tilde{f}(\boldsymbol{q})\tilde{f}(-\boldsymbol{q})\rangle \sim 1/q^{4-\eta}, \quad \langle(\Delta f)^2\rangle = \int\frac{d^2q}{(2\pi)^2}\tilde{G}(\boldsymbol{q}) \sim L^{2-\eta}$$

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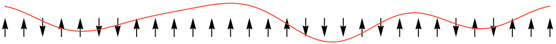
Fourier Monte Carlo (FMC)



- 4^{th} order anharmonicity is of “generalized squared-square” type

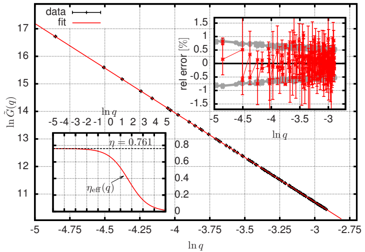
$$\mathcal{H}^{(a)}[\varphi] \sim \sum_{\boldsymbol{k}} B(\boldsymbol{k})\widetilde{S}(\boldsymbol{k})\widetilde{S}(-\boldsymbol{k}), \qquad \widetilde{S}(\boldsymbol{k}) \sim \sum_{\boldsymbol{q}} R(\boldsymbol{k},\boldsymbol{q})\tilde{f}(\boldsymbol{q})\tilde{f}(\boldsymbol{k}-\boldsymbol{q})$$

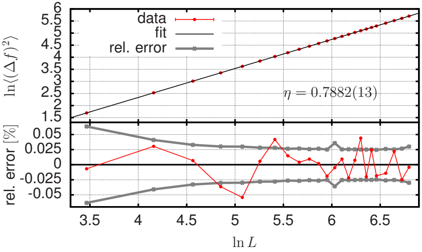
  so Fourier Monte Carlo is applicable.
- basic MC variables: discrete Fourier amplitudes $\tilde{f}(\boldsymbol{q}) = \sum_{\boldsymbol{x}} f(\boldsymbol{x})e^{-i\boldsymbol{q}\boldsymbol{x}}$
- MC move: pick random $\boldsymbol{q}_0$ and $\epsilon \in \mathbb{C}$ with $|\epsilon| \leq r(\boldsymbol{k})$ (NO reference to direct lattice!):

$$\tilde{f}(\boldsymbol{q}_0) \to \tilde{\varphi}(\boldsymbol{q}_0) + \epsilon, \quad \tilde{f}(-\boldsymbol{q}_0) \to \tilde{f}(-\boldsymbol{q}_0) + \epsilon^*$$

- **collective nonlocal moveset** is tailor-made for studying critical systems
- **long range interactions become diagonal** upon FT
- FMC can be tuned to drastically **suppress critical slowing down**

Results: 2-Point Correlation Function and Mean Squared Displacement





η	Method	Ref.
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Subleading **corrections to scaling** are extremely **important** for obtaining a reliable result!

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Reminder: Momentum Shell RG Prescription (K.G. Wilson 1972)

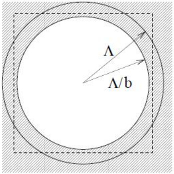
Denote effective Hamiltonian with couplings $\boldsymbol{K} \equiv (\kappa, K, \dots)$ at cutoff Λ by $\mathcal{H}^{\Lambda}_{\boldsymbol{K}}[f]$

- **Coarse-graining:** choose shell thickness parameter $b > 1$, separate f into "slow" and "fast" mode contributions

  $$\tilde{f}_{<}(\boldsymbol{k}) = \theta(\Lambda/b - |\boldsymbol{k}|)\tilde{f}(\boldsymbol{k}), \quad \tilde{f}_{>}(\boldsymbol{k}) = \theta(|\boldsymbol{k}| - \Lambda/b)\tilde{f}(\boldsymbol{k})$$

  and integrate out fast modes within momentum shell $\Lambda/b < |\boldsymbol{k}| \leq \Lambda$:

  $$e^{-\tilde{\mathcal{H}}^{\Lambda/b}_{\tilde{\boldsymbol{K}}}[f_{<}]} \equiv \int \mathcal{D}f_f e^{-\mathcal{H}^{\Lambda}_{\boldsymbol{K}}[f_{<}+f_{>}]}$$



- **Rescaling of lengths:** $\Lambda' = b\Lambda,\ \boldsymbol{k}' = b\boldsymbol{k},\ \boldsymbol{x}' = \boldsymbol{x}/b$
- **"wave function renormalization":** $\tilde{f}'(\boldsymbol{k}') \equiv z^{-1}(b, \boldsymbol{K})\tilde{f}(\boldsymbol{k})$ with $z(b, \boldsymbol{K}) = b^{d-[f]-\frac{\eta[\boldsymbol{K}]}{2}}$
- Result: **transformed effective Hamiltonian** $\mathcal{H}^{\Lambda}_{\boldsymbol{K}'}[f']$

$$e^{-\mathcal{H}^{\Lambda}_{\boldsymbol{K}'}[f']} \equiv \left[\int \mathcal{D}f_{>} e^{-\mathcal{H}^{\Lambda}_{\boldsymbol{K}}[f_{<}+f_{>}]}\right]_{\boldsymbol{k} \to \boldsymbol{k}'/b,\ \tilde{f}_{<}(\boldsymbol{k}) \to z(b,\boldsymbol{K})\tilde{f}'(\boldsymbol{k}')}$$

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Coarse Graining the Membrane Effective Hamiltonian

- consider configurations $f^{(\boldsymbol{k})} = f_<^{(\boldsymbol{k})} + f_>$ with slow "tracer" amplitudes

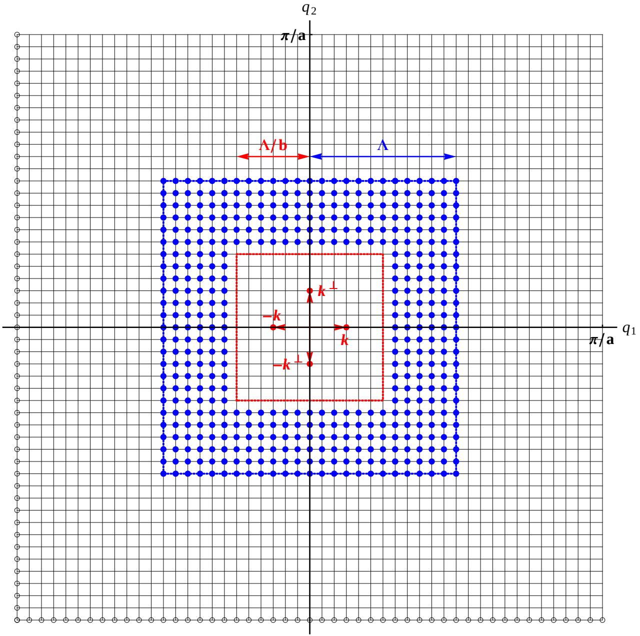
$$\tilde{f}_<^{(\boldsymbol{k})}(\boldsymbol{q}) = m\left(\delta_{\boldsymbol{q}-\boldsymbol{k}} + \delta_{\boldsymbol{q}-\boldsymbol{k}^\perp} + \delta_{\boldsymbol{q}+\boldsymbol{k}} + \delta_{\boldsymbol{q}+\boldsymbol{k}^\perp}\right), \qquad m \in \mathbb{R}, \qquad |\boldsymbol{k}| = |\boldsymbol{k}^\perp| < \Lambda/b,\ \boldsymbol{k}\cdot\boldsymbol{k}^\perp = 0$$

  Their "slow contribution" to membrane energy is a fourth order polynomial with $\boldsymbol{k}$-dependent coefficients in the real amplitude m:

$$\mathcal{H}_{\boldsymbol{K}}^{\Lambda}\left[f_<^{(t)}(m, \boldsymbol{k})\right] = 2\kappa k^4 \cdot m^2 + \frac{K}{2} k^4 \cdot m^4$$

(simple **dumbbell** $f_<^{(\boldsymbol{k})}(\boldsymbol{q}) \equiv m(\delta_{\boldsymbol{q}-\boldsymbol{k}} + \delta_{\boldsymbol{q}+\boldsymbol{k}})$ works in e.g. ϕ^4 model, but not here, since fourth order coefficient vanishes identically!)

Coarse Graining: “Cross” Tracer Configuration



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- for each $\boldsymbol{k}$ a multicanonical type of MC simulation based on the configurations $f^{(\boldsymbol{k})}$ yields the unnormalized probability distribution $P(m; \boldsymbol{k})$
- perform least squares fits of corresponding "free energies"

$$F(m; \boldsymbol{k}) = -\ln P_{\boldsymbol{K}}(m; \boldsymbol{k}) = b_0 + b_2(\boldsymbol{k})m^2 + b_4(\boldsymbol{k})m^4 + b_6(\boldsymbol{k})m^6 + b_8(\boldsymbol{k})m^8 + \ldots$$

- second level of least squares fits $b_2(\boldsymbol{k})$ and $b_4(\boldsymbol{k})$ as functions of $\boldsymbol{k}$ to the ansatz

$$b_2(\boldsymbol{k}) \equiv 2\tilde{\kappa} k^4 + O(k^6), \qquad b_4(\boldsymbol{k}) \equiv \frac{\tilde{K}}{2} k^4 + O(k^6)$$

  produces the sought-after CG relations

$$\kappa \to \tilde{\kappa}, \qquad K \to \tilde{K}$$

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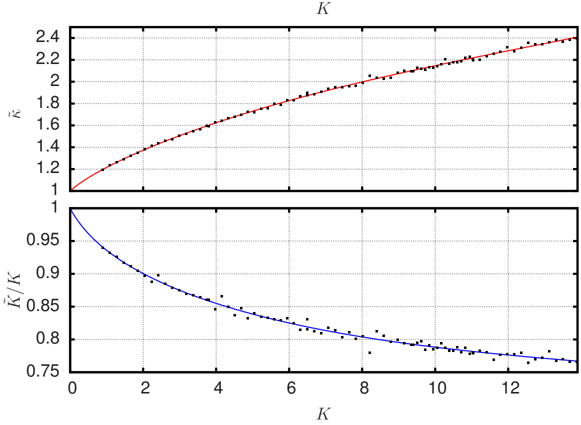
Coarse Graining: Resulting CG Coefficients $\tilde{\kappa}(K)$, $\tilde{K}(K)$

- For $K \to 0$ we must have $\tilde{\kappa}(K) \to \kappa = 1$ and $\tilde{K}(K) \to K$ i.e. $\tilde{K}(K)/K \to 1$:



(each data point of this example plot took 9 individual simulations)

- phenomenological fits of the functions $\tilde{\kappa}(K)$ and $\tilde{K}(K)/K$ using the ansatz

$$f(K) = 1 + a\ln(1 + b^2 K) + cK + dK^2 + eK^3$$

reduce noise and are convenient for subsequent numerical evaluation

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Numerical Determination of Fixed Point and Exponents η, ω

- Rescaling of lengths and further “wave function” renormalization:

$$\tilde{\boldsymbol{K}} \mapsto \begin{pmatrix} b^{-\eta(K)}\tilde{\kappa} \\ b^{2-2\eta(K)}\tilde{K} \end{pmatrix} =: \begin{pmatrix} \kappa' \\ K' \end{pmatrix} =: \boldsymbol{K}'$$

- invariance of $\kappa = 1.0$ defines function

$$\eta(K) \equiv \frac{\ln \tilde{\kappa}(K)}{\ln b}$$

- invariance of $K' \equiv K$ defines function

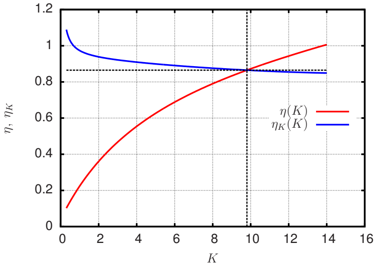
$$\eta_K(K) \equiv 1 + \frac{\ln \frac{\tilde{K}(K)}{K}}{2 \ln b}$$

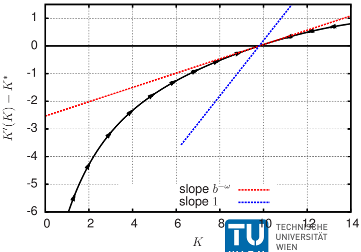
- At a FP $K' \equiv K \equiv K^*$ one has $\boxed{\eta(K^*) = \eta_K(K^*) \equiv \eta}$
- $K \mapsto K'(K)$ is analytic $\Rightarrow$ $K'(K^* + \delta K) \approx K^* + \mathcal{M} \cdot \delta K$ with slope

$$\mathcal{M} = \left.\frac{dK'(K)}{dK}\right|_{K=K^*}$$

- K is irrelevant: $0 < \mathcal{M} < 1$. Corresponding Wegner exponent:

$$\mathcal{M} \equiv b^{-\omega} \quad \Rightarrow \quad \boxed{\omega = -\frac{\ln \mathcal{M}}{\ln b}}.$$





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Results

- Note that $K^* = K^*(b)$ depends on b, since we have replaced the "exact" RG $\mathcal{R}_b$ by an effective transformation

$$\mathcal{R}^{\text{eff}}{}_b := \pi_{\text{eff}} \circ \mathcal{R}_b \circ \pi_{\text{eff}} .$$

where π_{eff} denotes the projection from ∞-dim. coupling constant space to the 2d hyperplane spanned by κ, K.

- $\mathcal{R}^{\text{eff}}{}_b$ does *not* strictly form a semi-group!

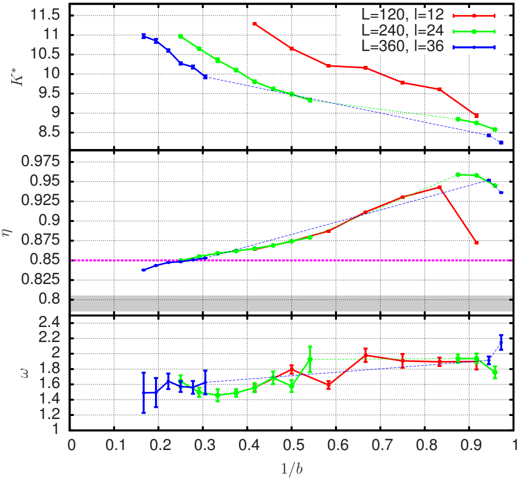
$$\mathcal{R}^{\text{eff}}{}_{b^2} \neq \mathcal{R}^{\text{eff}}{}_b \circ \mathcal{R}^{\text{eff}}{}_b$$

Equality may only be restored for $b \to 1$ or $b \to \infty$.
(A.T., PRB **79**, 036707 (2009); PRB **81**, 125135 (2010))

- For $b \to \infty$ (Bruce, Droz & Aharony 1974) we extrapolate

$$\eta = 0.822(1), \qquad \omega \approx 4/3$$

(first successful numerical estimate for ω)



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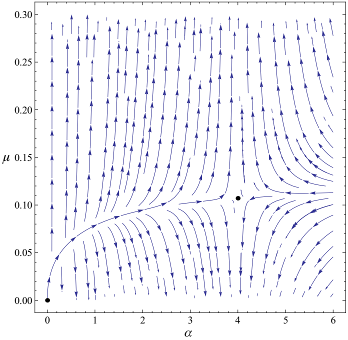
Take-Home Messages and Outlook

- Fourier Monte Carlo (FMC) is ideally suited to studying critical behavior in **lattice spin models with long range interactions**
- additional benefit: FMC can be easily tuned to **drastically suppress critical slowing down**
- ***b*-dependence of RG** results is frequently overlooked but worth studying; FMC seems to be the only method that allows to do this systematically
- the method not only reproduced a correct estimate for η but also allows in addition to announce the **first numerical estimate of exponent ω for a crystalline membrane**
- RG for crinkled phase of hexatic membranes is currently underway . . .



And finally I would like to say…

…thanks for your attention! :-)

Any questions?