Path Integration in Statistical Field Theory: from QM to Interacting Fermion Systems

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Methhods of Path Integration in Modern Physics
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- weakly coupled subsystems: perturbation theory
- if not: strongly coupled system

> properties can only be explained by
> strong correlations of subsystems

- example of strongly coupled systems:
  - ultra-cold atoms in optical lattices
  - high-temperature superconductors
  - statistical systems near phase transitions
  - strong interaction at low energies

- exactly soluble models (large symmetry, QFT, TFT)
- approximations

  mean field, strong coupling expansion, . . .
- restiction to effective degrees of freedom

  Born-Oppenheimer approximation, Landau-theory, . . .
- functional methods

  Schwinger-Dyson equations

  functional renormalization group equation
- numerical simulations

  lattice field theories = particular classical spin systems

  $\Rightarrow$ powerful methods of statistical physics and stochastics

Quantum mechanical system in thermal equilibrium

- Hamiltonian $\hat{H}:\mathcal{H}\mapsto\mathcal{H}$
- system in thermal equilibrium with heat bath

$$\text{canonical}\qquad \hat{\varrho}_\beta=\frac{1}{Z_\beta}\,\hat{K}(\beta),\quad \hat{K}(\beta)=\mathrm{e}^{-\beta\hat{H}},\quad \beta=\frac{1}{kT}$$

- normalizing partition function

$$Z_\beta=\operatorname{tr}\hat{K}(\beta)$$

- expectation value of observable $\hat{O}$ in ensemble

$$\langle\hat{O}\rangle_\beta=\operatorname{tr}\big(\hat{\varrho}_\beta\hat{O}\big)$$

- inner and free energy

$$U = \langle \hat{H} \rangle_\beta = -\frac{\partial}{\partial \beta} \log Z_\beta \quad , \quad F_\beta = -kT \log Z_\beta$$

$\Rightarrow$ all thermodynamic potentials, entropy $S = -\partial_T F, \ldots$

- specific heat

$$C_V = \langle \hat{H}^2 \rangle_\beta - \langle \hat{H} \rangle_\beta^2 = -\frac{\partial U}{\partial \beta} > 0$$

- system of particles: specify Hilbert space and $\hat{H}$

  identical bosons: symmetric states

  identical fermions: antisymmetric states

- traces on different Hilbert spaces

Path integral for partition function in quantum mechanics

- euclidean evolution operator $\hat{K}$ satisfies *diffusion* type equation

$$\hat{K}(\beta) = \mathrm{e}^{-\beta\hat{H}} \Longrightarrow \frac{\mathrm{d}}{\mathrm{d}\beta}\hat{K}(\beta) = -\hat{H}\hat{K}(\beta)$$

- compare with time-evolution operator and Schrödinger equation

$$\hat{U}(t) = \mathrm{e}^{-\mathrm{i}\hat{H}/\hbar} \Longrightarrow \mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\hat{U}(t) = \hat{H}\hat{U}(t)$$

- formally: $\hat{U}(t = -\mathrm{i}\hbar\beta) = \hat{K}(\beta)$, imaginary time
- $\hbar$ quantum fluctuations, kT thermal fluctuations

- evaluate trace in position space

$$\langle q|\,\mathrm{e}^{-\beta\hat{H}}|q'\rangle = K(\beta,q,q') \Longrightarrow Z_\beta = \int \mathrm{d}q\, K(\beta,q,q)$$

- "initial condition" for kernel: $\lim_{\beta\to 0} K(\beta,q,q') = \delta(q,q')$

free particle in d dimensions (Brownian motion)

$$\hat{H}_0 = -\frac{\hbar^2}{2m}\Delta \Longrightarrow K_0(\beta,q,q') = \left(\frac{m}{2\pi\hbar^2\beta}\right)^{d/2} \mathrm{e}^{-\frac{m}{2\hbar^2\beta}(q'-q)^2}$$

- Hamiltonian $\hat{H} = \hat{H}_0 + \hat{V}$ bounded from below $\Rightarrow$

$$\mathrm{e}^{-\beta(\hat{H}_0+\hat{V})} = s - \lim_{n\to\infty}\left(\mathrm{e}^{-\beta\hat{H}_0/n}\,\mathrm{e}^{-\beta\hat{V}/n}\right)^n, \quad \hat{V} = V(\hat{q})$$

- insert for every identity $\mathbb{1}$ in

$$\left(\mathrm{e}^{-\frac{\beta}{n}\hat{H}_0}\,\mathrm{e}^{-\frac{\beta}{n}\hat{V}}\right)\mathbb{1}\left(\mathrm{e}^{-\frac{\beta}{n}\hat{H}_0}\,\mathrm{e}^{-\frac{\beta}{n}\hat{V}}\right)\mathbb{1}\cdots\mathbb{1}\left(\mathrm{e}^{-\frac{\beta}{n}\hat{H}_0}\,\mathrm{e}^{-\frac{\beta}{n}\hat{V}}\right)$$

the resolution $\mathbb{1}=\int \mathrm{d}q\,|q\rangle\langle q| \;\Rightarrow$

$$\begin{aligned} K(\beta,q',q) &= \lim_{n\to\infty}\langle q'|\left(\mathrm{e}^{-\frac{\beta}{n}\hat{H}_0}\,\mathrm{e}^{-\frac{\beta}{n}\hat{V}}\right)^n|q\rangle \\ &= \lim_{n\to\infty}\int \mathrm{d}q_1\cdots\mathrm{d}q_{n-1}\prod_{j=0}^{j=n-1}\langle q_{j+1}|\,\mathrm{e}^{-\frac{\beta}{n}\hat{H}_0}\,\mathrm{e}^{-\frac{\beta}{n}\hat{V}}|q_j\rangle\;, \end{aligned}$$

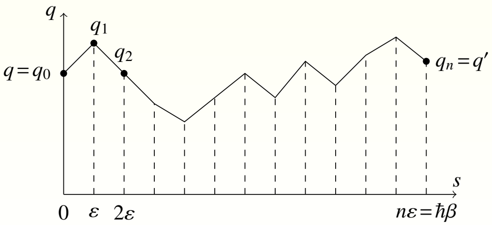
- initial and final positions $q_0=q$ and $q_n=q'$
- define small $\varepsilon=\hbar\beta/n$ and finally use

$$\begin{aligned} \mathrm{e}^{-\frac{\beta}{n}V(\hat{q})}|q_j\rangle &= |q_j\rangle\;\mathrm{e}^{-\frac{\beta}{n}V(q_j)} \\ \langle q_{j+1}|\,\mathrm{e}^{-\frac{\beta}{n}\hat{H}_0}|q_j\rangle &= \left(\frac{m}{2\pi\hbar\varepsilon}\right)^{d/2}\mathrm{e}^{-\frac{m}{2\hbar\varepsilon}(q_{j+1}-q_j)^2} \end{aligned}$$

- discretized "path integral"

$$K(\beta, q', q) = \lim_{n\to\infty} \int \mathrm{d}q_1 \cdots \mathrm{d}q_{n-1} \left(\frac{m}{2\pi\hbar\varepsilon}\right)^{n/2}$$
$$\cdot \exp\left\{-\frac{\varepsilon}{\hbar}\sum_{j=0}^{j=n-1}\left[\frac{m}{2}\left(\frac{q_{j+1}-q_j}{\epsilon}\right)^2 + V(q_j)\right]\right\}$$

- divide interval $[0, \hbar\beta]$ into n sub-intervals of length $\varepsilon = \hbar\beta/n$
- consider path $q(\tau)$ with sampling points $q(\tau = k\varepsilon) = q_k$



- Riemann sum in exponent approximates Riemann integral

$$S_E[q] = \int_0^\beta \mathrm{d}\tau \left(\frac{m}{2}\dot{q}^2(\tau) + V(q(\tau))\right)$$

- S_E is Euclidean action ($\propto$ action for imaginary time)
- integration over all sampling points $\stackrel{n\to\infty}{\longrightarrow}$ formal path integral $\mathcal{D}q$
- path integral with real and positive density

$$K(\beta, q', q) = \mathcal{C} \int_{q(0)=q}^{q(\hbar\beta)=q'} \mathcal{D}q \; \mathrm{e}^{-S_E[q]/\hbar}$$

- on diagonal = integration over all path $q \to q$

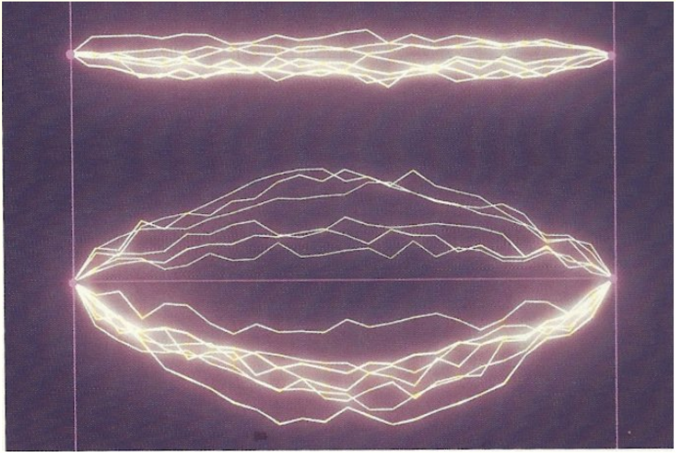
$$K(\beta, q, q) = \langle q|\,\mathrm{e}^{-\beta\hat{H}}|q\rangle = \mathcal{C}\int_{q(0)=q}^{q(\hbar\beta)=q} \mathcal{D}q\;\mathrm{e}^{-S_E[q]/\hbar}$$

- trace

$$\mathrm{tr}\;\mathrm{e}^{-\beta\hat{H}} = \int \mathrm{d}q\,\langle q|\,\mathrm{e}^{-\beta\hat{H}}|q\rangle = \mathcal{C}\oint_{q(0)=q(\hbar\beta)} \mathcal{D}q\;\mathrm{e}^{-S_E[q]/\hbar}$$

partition function $Z(\beta)$ integral over all periodic paths with period $\hbar\beta$.

- can construct well-defined Wiener-measure
  measure(differentable paths)$= 0$
  measure(continuous paths)$= 1$



exercise (Mehler formula)

show that the harmonic oscillator with Hamiltonian

$$\hat{H}_\omega = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}q^2} + \frac{m\omega^2}{2}q^2$$

has heat kernel

$$K_\omega(\beta, q', q) = \sqrt{\frac{m\omega}{2\pi\hbar\sinh(\hbar\omega\beta)}}\exp\left\{-\frac{m\omega}{2\hbar}\left[(q^2+q'^2)\coth(\hbar\omega\beta) - \frac{2qq'}{\sinh(\hbar\omega\beta)}\right]\right\}$$

- equation of euclidean motion $\ddot{q} = \omega^2 q$ has for given q, q' the solution

$$q(\tau) = q\cosh(\omega\tau) + \left(q' - q\cosh(\omega\beta)\right)\frac{\sinh(\omega\tau)}{\sinh(\omega\beta)}$$

- action

$$S = \frac{m}{2}\int_0^\beta (\dot{q}^2 + \omega^2 q^2) = \frac{m\omega}{2\sinh\omega\beta}\Big((q^2+q'^2)\cosh\omega\beta - 2qq'\Big)$$

- second derivative

$$\frac{\partial^2 S}{\partial q \partial q'} = -\frac{m\omega}{\sinh(\omega\beta)}$$

- semiclassical formula exact for harmonic oscillator

$$K(\beta, q', q) = \sqrt{-\frac{1}{2\pi}\frac{\partial^2 S}{\partial q \partial q'}}\,\mathrm{e}^{-S}$$

- yields above results for heat kernel

- diagonal elements

$$K_\omega(\beta, q, q) = \sqrt{\frac{m\omega}{2\pi\hbar\sinh(\hbar\omega\beta)}}\,\exp\left\{-\frac{2m\omega q^2}{\hbar}\frac{\sinh^2(\hbar\omega\beta/2)}{\sin(\hbar\omega\beta)}\right\}$$

- partition function

$$Z_\beta = \frac{1}{2\sinh(\hbar\omega\beta/2)} = \frac{\mathrm{e}^{-\hbar\omega\beta/2}}{1-\mathrm{e}^{-\hbar\omega\beta}} = \mathrm{e}^{-\hbar\omega\beta/2}\sum_{n=0}^{\infty}\mathrm{e}^{-n\hbar\omega\beta}$$

- evaluate trace with energy eigenbasis of $\hat{H} \Rightarrow$

$$Z(\beta) = \mathrm{tr}\,\mathrm{e}^{-\beta\hat{H}} = \langle n|\,\mathrm{e}^{-\beta\hat{H}}|n\rangle = \sum_n \mathrm{e}^{-\beta E_n}$$

- comparison of two sums $\Rightarrow$

$$E_n = \hbar\omega\left(n+\frac{1}{2}\right), \quad n\in\mathbb{N}$$

- position operator

$$\hat{q}(t) = \mathrm{e}^{it\hat{H}/\hbar}\hat{q}\,\mathrm{e}^{-it\hat{H}/\hbar}, \quad \hat{q}(0) = \hat{q}$$

- imaginary time $t = -i\tau \Rightarrow$ euclidean operator

$$\hat{q}_{\mathrm{E}}(\tau) = \mathrm{e}^{\tau\hat{H}/\hbar}\hat{q}\,\mathrm{e}^{-\tau\hat{H}/\hbar}, \quad \hat{q}_{\mathrm{E}}(0) = \hat{q}$$

- correlations at different $0 \leq \tau_1 \leq \tau_2 \leq \cdots \leq \tau_n \leq \beta$ in ensemble

$$\left\langle \hat{q}_{\mathrm{E}}(\tau_n) \cdots \hat{q}_{\mathrm{E}}(\tau_1) \right\rangle_\beta \equiv \frac{1}{Z(\beta)} \,\mathrm{tr}\left(\mathrm{e}^{-\beta\hat{H}} \hat{q}_{\mathrm{E}}(\tau_n) \cdots \hat{q}_{\mathrm{E}}(\tau_1) \right)$$

- consider thermal two-point function (now we set $\hbar = 1$)

$$\langle \hat{q}_{\mathrm{E}}(\tau_2)\hat{q}_{\mathrm{E}}(\tau_1)\rangle_\beta = \frac{1}{Z(\beta)} \,\mathrm{tr}\left(\mathrm{e}^{-(\beta-\tau_2)\hat{H}}\hat{q}\;\mathrm{e}^{-(\tau_2-\tau_1)\hat{H}}\hat{q}\;\mathrm{e}^{-\tau_1\hat{H}} \right)$$

- spectral decomposition: $|n\rangle$ orthonormal eigenstates of $\hat{H}$ $\Rightarrow$

$$\langle \dots \rangle_\beta = \frac{1}{Z(\beta)} \sum_n \mathrm{e}^{-(\beta-\tau_2)E_n} \langle n|\hat{q}\, \mathrm{e}^{-(\tau_2-\tau_1)\hat{H}} \hat{q}|n\rangle\, \mathrm{e}^{-\tau_1 E_n}$$

- insert $\mathbb{1} = \sum |m\rangle\langle m|$ $\Rightarrow$

$$\langle \dots \rangle_\beta = \frac{1}{Z(\beta)} \sum_{n,m} \mathrm{e}^{-(\beta-\tau_2+\tau_1)E_n}\, \mathrm{e}^{-(\tau_2-\tau_1)E_m} \langle n|\hat{q}|m\rangle\langle m|\hat{q}|n\rangle$$

- low temperature $\beta \to \infty$: contribution of excited states to $\sum_n(\dots)$ exponentially suppressed, $Z(\beta) \to \exp(-\beta E_0)$ $\Rightarrow$

$$\langle \hat{q}_\mathrm{E}(\tau_2)\hat{q}_\mathrm{E}(\tau_1)\rangle_\beta \overset{\beta\to\infty}{\longrightarrow} \sum_{m\geq 0} \mathrm{e}^{-(\tau_2-\tau_1)(E_m-E_0)} |\langle 0|\hat{q}|m\rangle|^2$$

- likewise

$$\langle \hat{q}_\mathrm{E}(\tau)\rangle_\beta \longrightarrow \langle 0|\hat{q}|0\rangle$$

- connected two-point function

$$\langle \hat{q}_\mathrm{E}(\tau_2)\hat{q}_\mathrm{E}(\tau_1)\rangle_{c,\beta} \equiv \langle \hat{q}_\mathrm{E}(\tau_2)\hat{q}_\mathrm{E}(\tau_1)\rangle_\beta - \langle \hat{q}_\mathrm{E}(\tau_2)\rangle_\beta \langle \hat{q}_\mathrm{E}(\tau_1)\rangle_\beta$$

- term with $m = 0$ in $\sum_m(\dots)$ cancels $\Rightarrow$ exponential decay with $\tau_1 - \tau_2$:

$$\lim_{\beta\to\infty} \langle \hat{q}_\mathrm{E}(\tau_2)\hat{q}_\mathrm{E}(\tau_1)\rangle_{c,\beta} = \sum_{m\geq 1} \mathrm{e}^{-(\tau_2-\tau_1)(E_m-E_0)}\, |\langle 0|\hat{q}|m\rangle|^2$$

- energy gap $E_1 - E_0$ and matrix element $|\langle 0|q|1\rangle|^2$ from

$$\langle \hat{q}_\mathrm{E}(\tau_2)\hat{q}_\mathrm{E}(\tau_1)\rangle_{c,\beta\to\infty} \longrightarrow \mathrm{e}^{-(E_1-E_0)(\tau_2-\tau_1)}\, |\langle 0|\hat{q}|1\rangle|^2\,, \quad \tau_2 - \tau_1 \to \infty$$

- for path-integral representation consider matrix elements

$$\left\langle q' \right| e^{-\beta\hat{H}} e^{\tau_2\hat{H}} \hat{q}\, e^{-\tau_2\hat{H}} e^{\tau_1\hat{H}} \hat{q}\, e^{-\tau_1\hat{H}} \left| q \right\rangle$$

- resolution of the identity and $\hat{q}|u\rangle = u|u\rangle$:

$$\langle \dots \rangle = \int \mathrm{d}v\mathrm{d}u \,\langle q'|\, e^{-(\beta-\tau_2)\hat{H}}|v\rangle v\langle v|\, e^{-(\tau_2-\tau_1)\hat{H}}|u\rangle u\langle u|\, e^{-\tau_1\hat{H}}|q\rangle$$

- path integral representations each propagator ($\beta > \tau_2 > \tau_1$):
  sum over paths with $q(0) = q$ and $q(\tau_1) = u$
  sum over paths with $q(\tau_1) = u$ and $q(\tau_2) = v$
  sum over paths with $q(\tau_2) = v$ and $q(\beta) = q'$
  multiply with intermediate positions $q(\tau_1)$ and $q(\tau_2)$
- $\int \mathrm{d}u\mathrm{d}v$: path integral over all paths with $q(0) = q$ and $q(\beta) = q'$

- insertion of $q(\tau_2)q(\tau_1$ in path integral

$$\langle \hat{q}_{\mathrm{E}}(\tau_2)\hat{q}_{\mathrm{E}}(\tau_1)\rangle_\beta = \frac{1}{Z(\beta)} \oint \mathcal{D}q\, \mathrm{e}^{-S_E[q]}\, q(\tau_2)q(\tau_1)$$

- similarly: thermal $n-$point correlation functions

$$\langle \hat{q}_{\mathrm{E}}(\tau_n)\cdots\hat{q}_{\mathrm{E}}(\tau_1)\rangle_\beta = \frac{1}{Z(\beta)} \oint \mathcal{D}q\, \mathrm{e}^{-S_E[q]}\, q(\tau_n)\cdots q(\tau_1)$$

conclusion

there exist a path integral representation for all equilibrium quantities, e.g.

- thermodynamic potentials, equation of state, correlation functions

real time: quantum mechanics

- action from mechanics

$$S = \int \mathrm{d}t \Big(\frac{m}{2}\dot{q}^2 - V(q)\Big)$$

- real time path integral

$$\langle q' | \, \mathrm{e}^{-it\hat{H}/\hbar} | q \rangle = \mathcal{C} \int_{q(0)=q}^{q(t)=q'} \mathcal{D}q \, e^{iS[q]/\hbar}$$

- correlation functions

$$\langle 0 | T \hat{q}(t_1) \hat{q}(t_2) | 0 \rangle = \mathcal{C} \int \mathcal{D}q \, e^{iS[q]/\hbar} q(t_1) q(t_2)$$

- oscillatory integrals

imaginary time: quantum statistics

- euclidean action

$$S_E = \int \mathrm{d}\tau \Big(\frac{m}{2}\dot{q}^2 + V(q)\Big)$$

- imaginary time path integral

$$\langle q' | \, \mathrm{e}^{-\beta\hat{H}/\hbar} | q \rangle = \mathcal{C} \int_{q(0)=q}^{q(\hbar\beta)=q'} \mathcal{D}q \, e^{-S_E[q]/\hbar}$$

- correlation functions

$$\langle \hat{q}_{\mathrm{E}}(\tau_1) \hat{q}_{\mathrm{E}}(\tau_2) \rangle_\beta = \mathcal{C} \int \mathcal{D}q \, e^{-S_E[q]/\hbar} q(\tau_1) q(\tau_2)$$

- exponentially damped integrals

- numerical simulations: discrete (euclidean) time
- system on time lattice = classical spin system

$$Z_\beta = \lim_{n\to\infty} \int \mathrm{d}q_1 \cdots \mathrm{d}q_n \left(\frac{m}{2\pi\hbar\varepsilon}\right)^{n/2} \mathrm{e}^{-S_E(q_1,\dots,q_n)/\hbar}$$

- expectation values of observables

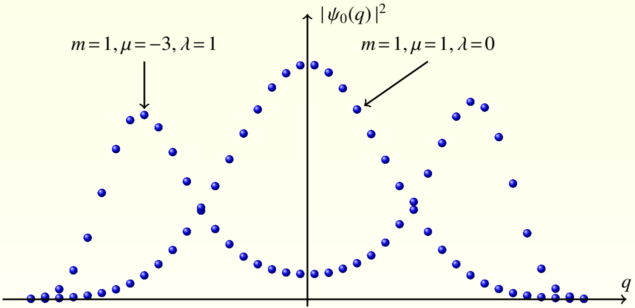
$$\int \mathrm{d}q_1 \dots \mathrm{d}q_n\, F(q_1,\dots,q_n)$$

high-dimensional integral (sometimes $n = 10^6$ required)

- curse of dimension: analytical and numerical approaches do not work
- stochastic methods, e.g. Monte-Carlo important sampling

what can be determined?

- energies, transitions amplitudes and wave functions in QM
- potentials, phase transitions, condensates and critical exponents
- bound states, masses and structure functions in particle physics . . .



$$\hat{H} = \frac{\hat{p}^2}{2m} + \mu\hat{q}^2 + \lambda\hat{q}^4$$

- Monte-Carlo simulation (Metropolis algorithm)
- square of the ground state wave function
- parameters in units of lattice constant ε

A. Wipf, Lecture Notes Physics 864 (2013)

exercise: harmonic chain

find free energy for periodic chain of coupled harmonic oscillators

$$H = \frac{1}{2m}\sum_{i=1}^{N} p_i^2 + \frac{m\omega^2}{2}\sum_i \left(q_{i+1}-q_i\right)^2, \quad q_i = q_{i+N}$$

- periodic $q(\tau) \Rightarrow$ may integrate by parts in

$$L_E = \frac{m}{2}\int \mathrm{d}\tau \left(\dot{q}^2 + \omega^2\left(q_{i+1}-q_i\right)^2\right)$$

- matrix notation

$$L_E = \frac{m}{2}\int \mathrm{d}\tau\, \boldsymbol{q}^T\left(-\frac{\mathrm{d}^2}{\mathrm{d}\tau^2} + A\right)\boldsymbol{q}, \quad A = \omega^2\left(2\delta_{ij} - \delta_{i,j+1} - \delta_{i,j-1}\right)$$

- hint: non-negative eigenvalues and orthonormal eigenvectors of A:

$$\omega_k = 2\,\omega \sin\frac{\pi k}{N} \quad \text{and} \quad \boldsymbol{e}_k$$

- expand $\boldsymbol{q}(\tau) = \sum c_k(\tau)\boldsymbol{e}_k$

$$L_E = \sum_k \frac{m}{2}\int \mathrm{d}\tau\,(\dot{c}_k^2 + \omega_k^2 c_k^2)$$

- N decoupled oscillators with frequencies $\omega_k \Rightarrow$

$$\langle \boldsymbol{q}|\,\mathrm{e}^{-\beta \hat{H}}|\boldsymbol{q}\rangle = \prod_k K_{\omega_k}(\beta, q_k, q_k)$$

- results for one-dimensional oscillator $\Rightarrow$

$$Z_\beta = \prod_k \frac{\mathrm{e}^{\beta\omega_k/2}}{\mathrm{e}^{\beta\omega_k} - 1} = \prod_k \frac{\mathrm{e}^{-\beta\omega_k/2}}{1 - \mathrm{e}^{-\beta\omega_k}}, \quad \omega_k = 2\,\omega \sin\frac{\pi k}{N}$$

- free energy contains zero-point energy

$$F_\beta = \frac{1}{2}\sum_k \hbar\omega_k + kT\sum_k \log\left(1 - \mathrm{e}^{-\hbar\omega_k/kT}\right)$$

- spin 0: scalar field (Higgs particle, inflaton,...)
- spin $\frac{1}{2}$: spinor field (electron, neutrinos, quarks, ...)
- spin 1: vector field (photon, W-bosons, Z-boson, gluons, ...)

a quick way from quantum mechanics to quantized scalar field theory:

- scalar field $\phi(t, \boldsymbol{x})$ satisfies Klein-Gordon type equation ($\hbar = c = 1$)

$$\Box\phi + V'(\phi) = 0$$

- Lagrangian = integral of Lagrangian density over space

$$L[\phi] = \int_{\text{space}} \mathrm{d}\boldsymbol{x}\, \mathcal{L}(\phi, \partial_\mu\phi), \quad \mathcal{L} = \frac{1}{2}\partial_\mu\phi\partial^\mu\phi - V(\phi)$$

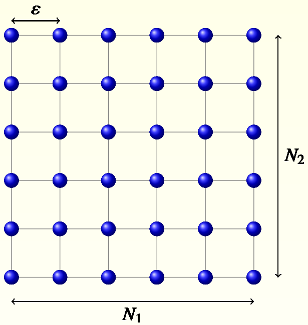
- momentum field, Legendre transform $\Rightarrow$ Hamiltonian (fixed time t)

$$\pi(\boldsymbol{x}) = \frac{\delta L}{\delta\dot\phi(\boldsymbol{x})} = \frac{\partial\mathcal{L}}{\partial\dot\phi(\boldsymbol{x})} = \dot\phi(\boldsymbol{x})$$

$$H = \int \mathrm{d}\boldsymbol{x}\,(\pi\dot\phi - L) = \int \mathrm{d}\boldsymbol{x}\,\mathcal{H}, \quad \mathcal{H} = \frac{1}{2}\pi^2 + \frac{1}{2}(\nabla\phi)^2 + V(\phi)$$

- free particle: $V \propto \phi^2 \Rightarrow$ Klein-Gordan $\Box\phi + m^2\phi = 0$
- infinitely many dof: one at each space point
- one of many possible regularizations: discretize space
- field theory on space lattice: $\boldsymbol{x} = \varepsilon\boldsymbol{n}$ with $\boldsymbol{n} \in \mathbb{Z}^{d-1}$

$$\phi(t,\boldsymbol{x}) \longrightarrow \phi_{\boldsymbol{x}=\varepsilon\boldsymbol{n}}(t) \quad , \quad \int \mathrm{d}\boldsymbol{x} \longrightarrow \varepsilon^{d-1}\sum_{\boldsymbol{n}}$$



- e.g. periodic bc
- lattice constant ε
- # of lattice sites $N = \prod N_i$
- linear extends $L_i = \varepsilon N_i$
- physical volume $V = \varepsilon^{d-1} N$

- finite hypercubic lattice in space

$$\boldsymbol{x} = \varepsilon\, \boldsymbol{n} \quad \text{with} \quad n_i \in \{1, 2, \dots, N_i\}$$

- continuum field $\phi(\boldsymbol{x}) \to$ lattice field $\phi_{\boldsymbol{x}}$
- integral $\to$ Riemann sum

$$\int \mathrm{d}\boldsymbol{x} \longrightarrow \varepsilon^{d-1} \sum_{\boldsymbol{n}}$$

- derivative $\to$ difference quotient

$$\frac{\partial \phi(\boldsymbol{x})}{\partial x_i} \longrightarrow (\partial_i \phi)_{\boldsymbol{x}}$$

- example: symmetric "lattice derivative"

$$(\partial_i \phi)_{\boldsymbol{x}} = \frac{\phi_{\boldsymbol{x}+\varepsilon \boldsymbol{e}_i} - \phi_{\boldsymbol{x}-\varepsilon \boldsymbol{e}_i}}{2\varepsilon}$$

- finite lattice $\to$ mechanical system with finite number of dof

$$H=\varepsilon^{d-1}\sum_{\boldsymbol{x}\in\text{lattice}}\Big(\frac{1}{2}\pi_{\boldsymbol{x}}^2+\frac{1}{2}(\partial\phi)_{\boldsymbol{x}}^2+V(\phi_{\boldsymbol{x}})\Big)$$

- path integral quantization known

$$\big\langle\{\phi'_{\boldsymbol{x}}\}\big|\,\mathrm{e}^{-\mathrm{i}\hat{H}/\hbar}\big|\{\phi_{\boldsymbol{x}}\}\big\rangle=\mathcal{C}\int\prod_{\boldsymbol{x}}\mathcal{D}\phi_{\boldsymbol{x}}\;\mathrm{e}^{\mathrm{i}S[\{\phi_{\boldsymbol{x}}\}]/\hbar}$$

- (formal) path integral over paths $\{\phi_{\boldsymbol{x}}(t)\}$ in configuration space

$$\phi_{\boldsymbol{x}}(0)=\phi_{\boldsymbol{x}}\quad\text{and}\quad\phi_{\boldsymbol{x}}(t)=\phi'_{\boldsymbol{x}},\quad\forall\,\boldsymbol{x}=\varepsilon\boldsymbol{n}$$

- high-dimensional quantum mechanical system with action

$$S[\{\phi_{\boldsymbol{x}}\}]=\int\mathrm{d}t\,\varepsilon^{d-1}\sum_{\boldsymbol{x}}\Big(\frac{1}{2}\dot{\phi}_{\boldsymbol{x}}^2-\frac{1}{2}(\partial\phi)_{\boldsymbol{x}}^2-V(\phi_{\boldsymbol{x}})\Big)$$

- canonical partition function

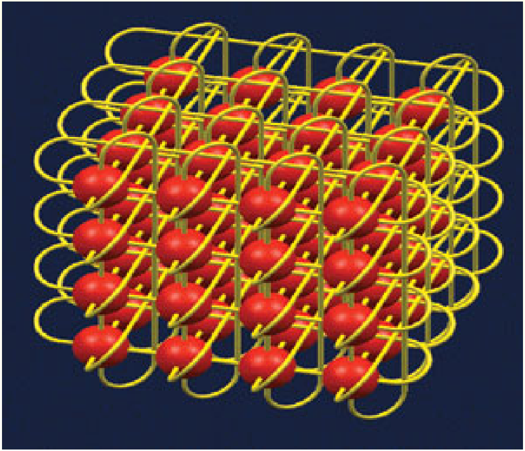
$$Z_\beta = \mathcal{C} \oint \prod_{\boldsymbol{x}} \mathcal{D}\phi_{\boldsymbol{x}}\ \mathrm{e}^{-S_E[\{\phi_{\boldsymbol{x}}\}]/\hbar}, \quad \phi_{\boldsymbol{x}}(\tau) = \phi_{\boldsymbol{x}}(\tau + \hbar\beta)$$

- real euclidean action

$$S_E[\{\phi_{\boldsymbol{x}}\}] = \int \mathrm{d}\tau\, \varepsilon^{d-1} \sum_{\boldsymbol{x}} \left(\frac{1}{2}\dot{\phi}_{\boldsymbol{x}}^2 + \frac{1}{2}(\partial\phi)_{\boldsymbol{x}}^2 + V(\phi_{\boldsymbol{x}})\right)$$

- path-integral well-defined after discretization of “time”
- convenient: same lattice constant ε in time and spatial directions
- replace $\tau \in [0, \hbar\beta] \longrightarrow \tau \in \{\varepsilon, 2\varepsilon, \dots, N_0\varepsilon\}$ with $N_0\varepsilon = \hbar\beta$
- lattice sites $(x^\mu) = (\tau, \boldsymbol{x}) = (\varepsilon n^\mu)$ with $n_\mu \in \{1, 2, \dots, N_\mu\}$

  $\Rightarrow$ d-dimensional hypercubic space-time lattice



lattice field ϕ_x defined on sites of space-time lattice Λ

- d-dimensional Euclid'sche space-time $\to$ lattice Λ, sites $x \in \Lambda$
- continuous field $\phi(x) \to$ lattice field ϕ_x, $x \in \Lambda$
  - finite lattice: extend in direction μ: $L_\mu = \varepsilon N_\mu$
    finite temperature: $L_1 = \cdots = L_{d-1} \gg L_0 \equiv \beta = 1/(kT)$
    scalar field periodic in imaginary time direction

$$\phi_{x=(x^0+\varepsilon N_0,\boldsymbol{x})} = \phi_{x=(x^0,\boldsymbol{x})} \Longrightarrow \text{temperature-dependence}$$

  - typically: also periodic in spatial directions
    $\Rightarrow$ identification $x^\mu \sim x^\mu + L_\mu$ (torus)
  - space-time volume $V = \varepsilon^d N_1 N_2 \cdots N_d$
  - some freedom in choice of lattice derivative (use symmetries)

dimensionless fields and couplings ($\hbar = c = 1$)

- natural units $\hbar = c = 1 \Rightarrow$ all units in powers of length L
- dimensionless action (unit L^0)

$$S_E = \int \mathrm{d}^d x \left(\frac{1}{2}(\partial\phi)^2 + \sum_a \lambda_a^{\mathrm{ph}}\,\phi^a \right)$$

- $\int \mathrm{d}^d x\,(\partial\phi)^2$ dimensionless $\Rightarrow [\partial\phi] = L^{-d/2} \Rightarrow [\phi] = L^{1-d/2}$
- $\lambda_a^{\mathrm{ph}} \int \mathrm{d}^d x\,\phi^a$ dimensionless $\Rightarrow [\lambda_a^{\mathrm{ph}}] = L^{-d-a+ad/2}$
- in particular $\lambda_2^{\mathrm{ph}} \propto m^2 \Rightarrow [m] = L^{-1}$
- 4 space-time dimensions $\Rightarrow \lambda_4^{\mathrm{ph}}$ dimensionless
- dimensionless lattice field and lattice constants ($x = \varepsilon n$)

$$\phi_x = \varepsilon^{1-d/2}\phi_n, \quad \lambda_a^{\mathrm{ph}} = \varepsilon^{-d-a+ad/2}\lambda_a$$

- lattice action with dimensionful quantities

$$S_L^{\mathrm{ph}} = \varepsilon^d \sum_x \left(\frac{1}{2} \left(\frac{\phi_{x+\varepsilon e_\mu} - \phi_{x-\varepsilon e_\mu}}{2\varepsilon} \right)^2 + \sum_a \lambda_a^{\mathrm{ph}} \phi_x^a \right)$$

$\Rightarrow$ lattice action with dimensionless quantities

$$S_L = \sum_n \left(\frac{1}{2} \left(\phi_{n+e_\mu} - \phi_{x-e_\mu} \right)^2 + \sum_a \lambda_a \phi_n^a \right)$$

- partition function

$$Z_\beta = \mathcal{C} \int \prod_{n=1}^{N_0 N_1 \cdots} \mathrm{d}\phi_n \; \mathrm{e}^{-S_L[\{\phi_n\}]}$$

- finite-dimensional well-defined integral (lattice regularization)
- lattice formulation without any dimensionful quantity
- processor knows numbers, not units!

- merely letting $\varepsilon \to 0$: no meaningful continuum limit
- λ_a must be changed as $\varepsilon \to 0$
- condition: dimensionful observables approach well-defined finite limits
- existence of such continuum limit not guaranteed
- example: consider correlation length in

$$\langle \phi(n)\phi(m)\rangle_c \propto \mathrm{e}^{-|n-m|/\xi}, \quad \frac{1}{\xi} = m = \text{dimnsionless mass}$$

- ξ depends on dimensionless couplings $\xi = \xi(\lambda_a)$
- relates to (given) dimensionful mass $m^{\mathrm{ph}} = 1/(\varepsilon\xi) \Rightarrow \varepsilon$
- m^{ph} from experiment, $\xi(\lambda_a)$ measured on lattice
- renormalization: keep m^{ph} (and further observables) fixed $\Rightarrow \lambda_a$

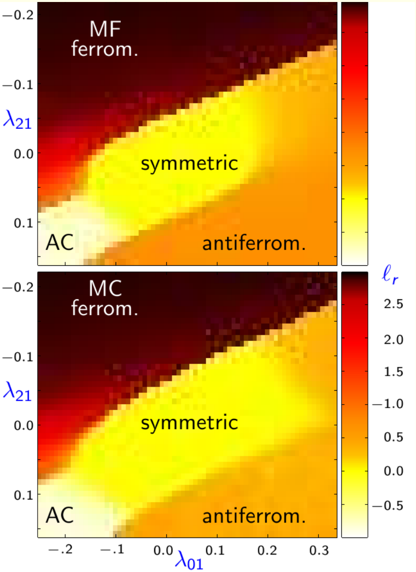
- extend of physical objects $\gg$ separation of lattice points
- extend of physical objects $\ll$ box size
- conditions (scaling window)
  - small discretization effects $\xi \gg 1$
  - small finite size effects $\xi \ll N_\mu$
  - strict continuum limit: $\xi \to \infty$
- 2'nd order phase transition required in system with $N_{\text{spatial}} \to \infty$
- theory renormalizable: only a small number of λ_a must be tuned
- relevant renormalizable field theories
  - non-Abelian gauge theories in $d \leq 4$
  - scalar field theories in $d < 4$
  - four-Fermi theories in $d \leq 3$
  - non-linear sigma-models in $d \leq 3$
  - Einstein-gravity in $d \leq 4$ (???)

- input in simulations: only a few observables (masses)
- simulate with stochastic algorithms in scaling window
- repeat simulations with same observables but decreasing ε
- output: many (dimensionful) observables
- extrapolate to $\varepsilon \to 0$
- if theory renormalizable: converge to a continuum limit as $\varepsilon \to 0$
- finite temperature: N_0 given, ε from matching to observable $\Rightarrow \beta = \varepsilon N_0$.

  $\Rightarrow$ temperature dependence of
  - free energy
  - condensates
  - pressure, densities
  - free energy of two static charges (confinement)
  - phase diagram
  - screening effects
  - correlations in heat bath, ...

- path integral for finite temperature QFT = classical spin model
- no non-commutative operators, instead: path or functional integration over fields
- scalar field: assign $\phi_n \in \mathbb{R}$ to each lattice site
- sigma models: $\phi_n \in$ Sphere
- discrete spin models: $\phi_n \in$ discrete group
- example: Potts-model: $\phi_n \in \mathbb{Z}_q$

  figures: 3−state Potts-type model



electron, muon, quarks, ...are described by 4-component spinor field $\psi_\alpha(x)$

- metric tensor in Minkowski space-time

$$(\eta_{\mu\nu}) = \text{diag}(1, -1, -1, -1)$$

- 4×4 gamma-matrices

$$\gamma^0, \dots, \gamma^3, \quad \{\gamma^\mu, \gamma^\nu\} = 2\eta^{\mu\nu}\mathbb{1}$$

- covariant Dirac equation for free massive fermions

$$(\mathrm{i}\not{\partial} - m)\,\psi(x) = 0, \quad \not{\partial} = \gamma^\mu \partial_\mu$$

- Euler-Lagrange equation of invariant action

$$S = \int \mathrm{d}^4 x \bar{\psi}(\mathrm{i}\not{\partial} - m)\psi, \quad \bar{\psi} = \psi^\dagger \gamma^0 \Longrightarrow \pi_\psi = -\mathrm{i}\psi^\dagger$$

- quantization: $\psi(x) \to \hat{\psi}(x)$
- satisfies anti-commutation relation

$$\{\hat{\psi}_\alpha(t,\boldsymbol{x}),\hat{\psi}^\dagger_\beta(t,\boldsymbol{y})\} = \delta_{\alpha\beta}\delta(\boldsymbol{x}-\boldsymbol{y})$$

- Hamilton operator: $\beta=\gamma^0,\ \boldsymbol{\alpha}=\gamma^0\boldsymbol{\gamma}$:

$$\hat{H} = \int \mathrm{d}\boldsymbol{x}\ \hat{\psi}^\dagger(\boldsymbol{x})(\hat{h}\hat{\psi})(\boldsymbol{x}), \quad \hat{h} = \mathrm{i}\,\boldsymbol{\alpha}\cdot\nabla + m\,\beta$$

- derive path integral representation of partition function

$$Z_\beta = \mathrm{tr}\,\mathrm{e}^{-\beta\hat{H}}$$

- leads to imaginary time path integral
- replace $t \to -\mathrm{i}\tau$ and

$$\gamma^0_{\mathrm{E}} = \gamma^0 \quad \text{and} \quad \gamma^i_{\mathrm{E}} = \mathrm{i}\gamma^i$$

- ACR with euclidean metric

$$\{\gamma_E^\mu, \gamma_E^\nu\} = 2\delta^{\mu\nu}\mathbb{1}, \qquad \gamma_E^\mu \text{ hermitean}$$

- lattice regularization (drop index E)

  space-time $\mathbb{R}^4 \to$ finite (hypercubic) lattice Λ
  continuum field $\psi(x)$ on $\mathbb{R}^4 \to$ lattice field ψ_x

- expected path integral

$$Z_\beta = \mathrm{tr}_{\mathrm{reg}}\, \mathrm{e}^{-\beta\hat{H}} = \mathcal{C} \oint \prod_{\alpha,x\in\Lambda} \mathrm{d}\psi^\dagger_{\alpha,x}\, \mathrm{d}\psi_{\alpha,x}\; \mathrm{e}^{-S_L[\psi,\psi^\dagger]}$$

- integration over anti-periodic fields (ACR for ψ, see below)

$$\psi_{\boldsymbol{x}}(\tau+\beta) = -\psi_{\boldsymbol{x}}(\tau), \quad \text{also on time lattice}$$

- S_L some lattice regularization of

$$S_E = \int \mathrm{d}^d x\, \psi^\dagger(\mathrm{i}\partial\!\!\!/ + \mathrm{i}m)\psi$$

- quantized scalar field obey equal-time CR

$$[\hat{\phi}(t,\boldsymbol{x}),\hat{\phi}(t,\boldsymbol{y})]=0,\quad \boldsymbol{x}\neq\boldsymbol{y}$$

$\Rightarrow$ commuting fields in path integral

$$[\phi(x),\phi(y)]=0,\quad \forall x,y$$

- quantized fermion field obey equal-time ACR

$$\{\hat{\psi}_\alpha(t,\boldsymbol{x}),\hat{\psi}^\dagger_\beta(t,\boldsymbol{y})\}=0,\quad \boldsymbol{x}\neq\boldsymbol{y}\ ,$$

$\Rightarrow$ anti-commuting fields in path integral

$$\{\psi_\alpha(x),\psi^\dagger_\beta(y)\}=0,\quad \forall x,y$$

- variables $\{\psi_{\alpha,n},\psi^\dagger_{\alpha,n}\}$ in fermion path integral: Grassmann variables

- free theories have quadratic action
  Gaussian integrals with $A = A^T$ positive matrix; exercise $\Rightarrow$

$$\int \prod_{n=1}^{N} \mathrm{d}\phi_n \, \exp\Big(-\frac{1}{2}\sum \phi_n A_{nm} \phi_m\Big) = \frac{(2\pi)^{n/2}}{\sqrt{\det A}}$$

- what do we get for fermions?
- simplify notation: $\psi_{\alpha,n} \equiv \eta_i$ and $\psi^\dagger_{\alpha,n} \equiv \bar\eta_i$ with $i = 1, \dots, m$
- objects $\{\eta_i, \bar\eta_i\}$ form complex Grassmann algebra:

$$\{\eta_i, \eta_j\} = \{\bar\eta_i, \bar\eta_j\} = \{\eta_i, \bar\eta_j\} = 0 \Longrightarrow \eta_i^2 = \bar\eta_i^2 = 0$$

Grassmann integration defined by ($a, b \in \mathbb{C}$)

$$\int \text{ linear}\,, \quad \int \mathrm{d}\eta_i (a + b\,\eta_i) = b, \quad \int \mathrm{d}\bar\eta_i (a + b\,\bar\eta_i) = b$$

- Grassmann integrals with

$$\mathcal{D}\bar{\eta}\mathcal{D}\eta \equiv \prod_{i=1}^{m} \mathrm{d}\bar{\eta}_i \mathrm{d}\eta_i$$

- free fermions $\Rightarrow$ Gaussian Grassmann integral

$$Z = \int \mathcal{D}\bar{\eta}\mathcal{D}\eta\, \mathrm{e}^{-\bar{\eta}A\eta}, \quad \bar{\eta}A\eta = \sum_{i,j} \bar{\eta}_i A_{ij} \eta_j$$

- expand exponential function: $\int \mathcal{D}\bar{\eta}\mathcal{D}\eta \left(\bar{\eta}A\eta\right)^k = 0$ for $k \neq m$
- remaining contribution (use $\bar{\eta}_i^2 = 0$)

$$\begin{aligned}
\frac{1}{n!}\int \mathcal{D}\bar{\eta}\mathcal{D}\eta\, (\bar{\eta}A\eta)^m &= \int \mathcal{D}\bar{\eta}\mathcal{D}\eta \sum_{i_1,\dots,i_m} (\bar{\eta}_1 A_{1i_1}\eta_{i_1})\cdots(\bar{\eta}_m A_{mi_m}\eta_{i_m}) \\
&= \int \mathcal{D}\bar{\eta}\mathcal{D}\eta \prod_i (\bar{\eta}_i\eta_i) \sum_{i_1,\dots,i_m} \varepsilon_{i_1\dots i_m} A_{1i_1}\cdots A_{mi_m} \\
&= (-1)^m \int \prod_i (\mathrm{d}\bar{\eta}_i\bar{\eta}_i\, \mathrm{d}\eta_i\eta_i)\, \det A = (-1)^m \det A
\end{aligned}$$

- simple formula

$$\int \mathcal{D}\bar{\eta}\mathcal{D}\eta\ \mathrm{e}^{-\bar{\eta}A\eta} = \det A$$

- generalization: generating function

$$Z(\bar{\alpha},\alpha) = \int \mathcal{D}\bar{\eta}\mathcal{D}\eta\ \mathrm{e}^{-\bar{\eta}A\eta+\bar{\alpha}\eta+\bar{\eta}\alpha} = \left(\mathrm{e}^{-\bar{\alpha}A^{-1}\alpha}\right)\det A$$

- expand in powers of $\bar{\alpha}$, $\alpha \Rightarrow$

$$\langle\bar{\eta}_i\eta_j\rangle \equiv \frac{1}{Z}\int \mathcal{D}\bar{\eta}\mathcal{D}\eta\ \mathrm{e}^{-\bar{\eta}A\eta}\,\bar{\eta}_i\eta_j = (A^{-1})_{ij}$$

- application to Dirac fields: above partition function

$$Z_\beta = \oint \mathcal{D}\bar{\psi}\mathcal{D}\psi\ \mathrm{e}^{-S_L}, \quad \mathcal{D}\bar{\psi}\mathcal{D}\psi = \prod_{\alpha,n}\mathrm{d}\psi^\dagger_{\alpha,n}\,\mathrm{d}\psi_{\alpha,n}$$

- dimensionless field and couplings

$$S_L = \sum_{n\in\Lambda} \psi_n^\dagger(\mathrm{i}\partial\!\!\!/_{nm} + \mathrm{i}m\delta_{nm})\psi_n = \sum_n \bar{\psi}_n D_{nm}\psi_m$$

- lattice partition function

$$Z_\beta = \mathcal{C}\,\det D$$

- expectation value in canonical ensemble

$$\langle\hat{A}\rangle_\beta = \frac{1}{Z_\beta}\oint \mathcal{D}\bar{\psi}\mathcal{D}\psi\, A(\bar{\psi},\psi)\; \mathrm{e}^{-S_L(\psi,\bar{\psi})}$$

- formula for complex scalar field

$$Z_\beta = \oint \mathcal{D}\phi\mathcal{D}\bar{\phi}\,\exp\left(-\sum \bar{\phi}_m C_{mn}\phi_n\right) \propto \frac{1}{\det C}$$

- boson fields: periodic in imaginary time

  fermion fields: anti-periodic in imaginary time

- neutral scalars (+: periodic bc)

$$S_E = \frac{1}{2}\int \phi(-\Delta + m^2)\,\phi \Longrightarrow F_\beta = \frac{kT}{2}\log\det{}_+(-\Delta + m^2) + \dots$$

- Dirac fermions (−: anti-periodic bc)

$$S_E = \int \psi^\dagger(\mathrm{i}\partial\!\!\!/ + \mathrm{i}m)\,\psi \Longrightarrow F_\beta = -2kT\log\det{}_-(-\Delta + m^2) + \dots$$

exercise

Try to prove the results for fermions (including sign and overall factor)

zeta-function for second order operator $A > 0$

$$\zeta_A(s) = \sum_n \lambda_n^{-s}, \quad \text{eigenvalues } \lambda_n$$

- absolute convergent series in half-plane $\Re(s) > d/2$
- meromorphic analytic continuation, analytic in neighborhood of $s = 0$
- defines $\zeta-$function regularized determinant Dowker, Hawking

$$\log\det A = \mathrm{tr}\log A = \sum \log\lambda_n = -\frac{\mathrm{d}\zeta_A(s)}{\mathrm{d}s}\Big|_{s=0}$$

- correct for matrices
- Mellin transformations

$$\int_0^\infty \mathrm{d}t\, t^{s-1} e^{-t\lambda} = \Gamma(s)\,\lambda^{-s}$$

$\Rightarrow$ relation to heat kernel

$$\zeta_A(s) = \sum_n \frac{1}{\Gamma(s)} \int_0^\infty \mathrm{d}t\, t^{s-1} e^{-t\lambda_n} = \frac{1}{\Gamma(s)} \int_0^\infty \mathrm{d}t\, t^{s-1}\,\mathrm{tr}\left(\mathrm{e}^{-tA}\right)$$

- coordinate representation

$$\zeta_A(s) = \frac{1}{\Gamma(s)} \int_0^\infty \mathrm{d}t\, t^{s-1} \int \mathrm{d}x\, K(t;x,x), \quad K(t) = \mathrm{e}^{-tA}$$

- heat kernel of $A = -\Delta + m^2$ on cylinder $[0,\beta] \times \mathbb{R}^{d-1}$

$$K^\pm(t;x,x') = \frac{\mathrm{e}^{-m^2 t}}{(4\pi t)^{d/2}} \sum_{n\in\mathbb{Z}} (\pm 1)^n\, \mathrm{e}^{-\left\{(\tau-\tau'+n\beta)^2+(\boldsymbol{x}-\boldsymbol{x}')^2\right\}/4t}$$

- integrate over diagonal elements

$$\zeta_A^\pm(s) = \frac{\beta V}{(4\pi)^{d/2}\Gamma(s)} \int \mathrm{d}t\, t^{s-1-d/2}\, \mathrm{e}^{-m^2 t} \sum_{n=-\infty}^{\infty} (\pm)^n\, \mathrm{e}^{-n^2\beta^2/4t}$$

- Jacobi theta function

- integral representation of Kelvin functions

$$\int_0^\infty \mathrm{d}t\, t^a\, \mathrm{e}^{-bt-c/t} = 2\left(\frac{c}{b}\right)^{(a+1)/2} K_{a+1}\left(2\sqrt{bc}\right)$$

$\Rightarrow$ series representation; in $d=4$

$$\zeta_A^{\pm}(s) = \frac{\beta V}{16\pi^2}\frac{m^{4-2s}}{\Gamma(s)}\left(\Gamma(s-2) + 4\sum_1^\infty (\pm)^n \left(\frac{nm\beta}{2}\right)^{s-2} K_{2-s}(nm\beta)\right)$$

- identities

$$\frac{\Gamma(s-2)}{\Gamma(s)} = \frac{1}{(s-1)(s-2)} \quad \text{and} \quad \frac{1}{\Gamma(s)} = s + O(s^2)$$

- derivative at $s = 0 \Rightarrow$

$$F_\beta^\pm = -\frac{m^4 V \mathcal{C}_\pm}{128\pi^2}\left(3 - 2\log\frac{m^2}{\mu^2} + 64\sum_{n=1,2\dots}(\pm)^n \frac{K_2(nm\beta)}{(nm\beta)^2}\right)$$

- real scalars $\mathcal{C}_+ = 1$, complex fermions $\mathcal{C}_- = -4$
- well-known results for massless particles $K_2(x) \sim 2/x^2$

$$\lim_{m\to 0} f^+(\beta) = -\frac{\pi^2}{90}T^4 \quad , \quad \lim_{m\to 0} f^-(\beta) = -\frac{2}{45\pi^2}T^4$$

questions

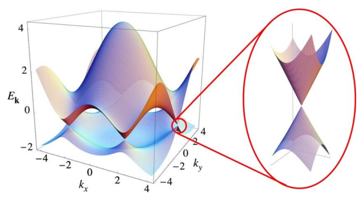
Why is there a relative factor of 4? What is the free energies of complex scalars, Majorana fermions and photons. What is free energy of complex fermions in d dimensions?

condensed matter systems in $d = 2 + 1$

- tight binding approximation for small excitation energies
- honeycomb lattice for graphen (GN): 2 atoms in every cell, 2 Dirac points $\Rightarrow$ 4-component spinor field
- interaction-driven transition metal $\leftrightarrow$ insolator
- long rang order: AF, CDW, ...
- interacting fermions (symmetries!)

condensed matter systems in $d = 1 + 1$

- conducting polymers (Trans- and Cis-polyacetylen) Su, Schrieffer, Heeger
- quasi-one-dimensional inhomogeneous superconductor Mertsching, Fischbeck



relativistic dispersion-relations for electronic excitations on honeycomb lattice

from Castro Neto et al.

- irreducible spinor in two and three dimensions has 2 components
- $\mathrm{N_f}$ species (flavours) of spinors, $\Psi = (\psi_1, \dots, \psi_{\mathrm{N_f}})$
- relativistic fermions

$$\mathcal{L}_{\mathrm{GN}} = \bar{\Psi}\mathrm{i}\partial\!\!\!/\Psi + \mathrm{i}m\bar{\Psi}\Psi + \mathcal{L}_{\mathrm{Int}}(\Psi, \bar{\Psi}), \quad \text{e.g. } \bar{\Psi}\Psi = \sum \bar{\psi}_i\psi_i$$

- parity invariant models

$$\mathcal{L}_{\mathrm{Int}} = \frac{g^2_{\mathrm{GN}}}{2\mathrm{N_f}}(\bar{\Psi}\Psi)(\bar{\Psi}\Psi) \quad \text{scalar-scalar, Gross-Neveu}$$

$$\mathcal{L}_{\mathrm{Int}} = -\frac{g^2_{\mathrm{Th}}}{2\mathrm{N_f}}(\bar{\Psi}\gamma^\mu\Psi)(\bar{\Psi}\gamma_\mu\Psi) \quad \text{vector-vector, Thirring}$$

$$\mathcal{L}_{\mathrm{Int}} = \frac{g^2_{\mathrm{PS}}}{2\mathrm{N_f}}(\bar{\Psi}\gamma_*\Psi)(\bar{\Psi}\gamma_*\Psi) \quad \text{pseudoscalar-pseudoscalar}$$

- in even dimensions $\gamma_* \propto \prod \gamma_\mu$
- Hubbard-Stratonovich trick with scalar, vector and pseudscalar field

- combinations thereof in $d = 4$
  non-renormalizable Fermi theory of weak interaction
  effective models for chiral phase transition in QCD (Jona Lasino)
- 2 spacetime dimensions: $[g] = L^0$
  - massless ThM: soluble — Thirring
  - massless ThM in curved space with μ: soluble — Sachs+AW, ...
  - GNM: asymptotically free, integrable — Gross-Neveu, Coleman, ...
- 3 spacetime dimensions: $[g] = Ls$
  - not renormalizable in PT
  - renormalizable in large-N expansion — Gawedzki, Kupiainen; Park, Rosenstein, Warr
  - interacting UV fixed point $\to$ asymptotically safe — de Veiga; da Calen; Gies, Janssen
  - can exhibit parity breaking at low T
- lattice theories:
  - generically: sign problem even for $\mu = 0$
  - partial solution of sign problem — Schmidt, Wellegehausen, Lenz, AW

with J. Lenz, L. Panullo, M. Wagner and B. Wellegehausen

- GN shows breaking of discrete chiral symmetry
- order parameter $\mathrm{i}\Sigma = \langle\bar\Psi\Psi\rangle$

$$\psi_a \to \mathrm{i}\gamma_*\psi_a,\quad \bar\psi_a \to \mathrm{i}\bar\psi_a\gamma_* \Longrightarrow \mathrm{i}\Sigma = \langle\bar\Psi\Psi\rangle \to -\langle\bar\Psi\Psi\rangle$$

- equivalent formulation with auxiliary scalar field Hubbard-Stratonovich transformation

$$\mathcal{L}_{\mathrm{GN}} = \mathcal{L}_\sigma = \bar\Psi\big(\mathrm{i}D\otimes\mathbb{1}_{\mathrm{N_f}}\big)\Psi + \frac{\mathrm{N_f}}{2g}(\bar\Psi\Psi)^2$$

$$\mathcal{L}_\sigma = \bar\Psi\big(\mathrm{i}D\otimes\mathbb{1}_{\mathrm{N_f}}\big)\Psi + \lambda\mathrm{N_f}\,\sigma^2,\qquad D = \partial\!\!\!/ - \sigma \neq D^\dagger$$

- conserved fermion charge

$$Q = \int_{\text{space}} \mathrm{d}\boldsymbol{x}\, j^0 = \int_{\text{space}} \mathrm{d}\boldsymbol{x}\, \psi^\dagger \psi$$

- partition function of grand canonical ensemble

$$Z_{\beta,\mu} = \mathrm{tr}\, \mathrm{e}^{-\beta(\hat{H}-\mu\hat{Q})},$$

- functional integral with above $\mathcal{L}_\sigma$ wherein

$$D = \partial\!\!\!/ + \sigma + \mu\gamma^0$$

- expectation values

$$\langle\mathcal{O}\rangle = \frac{1}{Z_{\beta,\mu}} \int \mathcal{D}\bar{\psi}\mathcal{D}\psi\mathcal{D}\sigma\ \mathrm{e}^{-S_\sigma}\,\mathcal{O}$$

- fermion integral in

$$Z_{\beta,\mu} = \int \mathcal{D}\bar{\psi}\mathcal{D}\psi\mathcal{D}\sigma \; \mathrm{e}^{-S_\sigma[\sigma,\psi,\bar{\psi}]} = \int \mathcal{D}\sigma \; \mathrm{e}^{-\mathrm{N_f} S_{\text{eff}}[\sigma]}$$

- $\mathrm{N_f}$ fermion species couple identically to auxiliary field $\Rightarrow$

$$\det\left(\mathrm{i}D \otimes \mathbb{1}\right) = (\det \mathrm{i}D)^{\mathrm{N_f}}$$

- ψ anti-periodic in imaginary time, σ periodic
- effective action after fermion integral

$$S_{\text{eff}} = \lambda \int \mathrm{d}^2x\, \sigma^2 - \log(\det \mathrm{i}D)$$

- Ward identity (lattice regularization)

$$\frac{1}{Z_{\beta,\mu}} \int \mathcal{D}\psi\, \mathcal{D}\bar{\psi}\, \mathcal{D}\sigma \, \frac{\mathrm{d}}{\mathrm{d}\sigma(x)} \left(\mathrm{e}^{-S[\sigma,\psi,\psi^\dagger]} \right) = -\left\langle \frac{\mathrm{d}S}{\mathrm{d}\sigma(x)} \right\rangle = 0$$

- exact relation

$$\Sigma \equiv -\mathrm{i}\langle\bar{\psi}(x)\psi(x)\rangle = \frac{\mathrm{N_f}}{g^2}\langle\sigma(x)\rangle$$

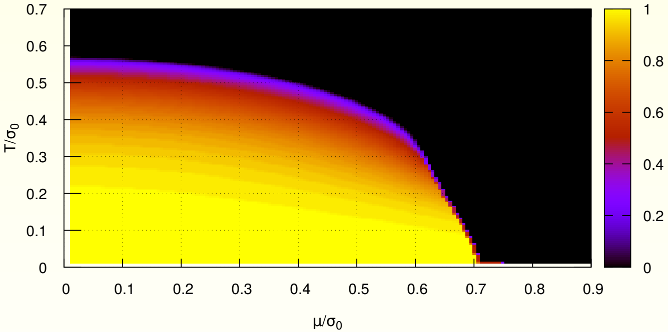
- for $\mathrm{N_f} \to \infty$ saddle point (steepest descend) approximation

$$Z_{\beta,\mu} = \int \mathcal{D}\sigma\, \mathrm{e}^{-\mathrm{N_f} S_{\text{eff}]}[\sigma]} \stackrel{\mathrm{N_f}\to\infty}{\longrightarrow} \mathrm{e}^{-\mathrm{N_f}\min S_{\text{eff}}[\sigma]}$$

- translation invariance $\Rightarrow$ minimizing σ constant: $S_{\text{eff}} = (\mathrm{N_f}\beta L)\, U_{\text{eff}}$

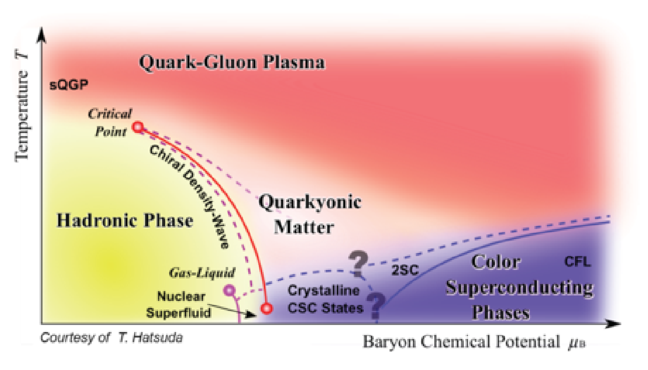
$$U_{\text{eff}} = \frac{\sigma^2}{4\pi}\left(\log\frac{\sigma^2}{\sigma_0} - 1\right) - \frac{1}{\pi}\int_0^\infty \mathrm{d}p\, \frac{p^2}{\varepsilon_p}\left(\frac{1}{1+\mathrm{e}^{\beta(\varepsilon_p+\mu)}} + \frac{1}{1+\mathrm{e}^{\beta(\varepsilon_p-\mu)}}\right)$$

- one-particle energies $\epsilon_p = \sqrt{p^2+\sigma^2}$
- IR-scale $\sigma_0 = \langle\sigma\rangle_{T=\mu=0}$



- symmetric phase for large T, μ
- homogeneously broken phase for small T, μ Wolff, Barducci
- special points: $(T_c, \mu) = (e^\gamma/\pi, 0)$, $(T, \mu_c) = (0, 1/\sqrt{2})$
- Lifschitz-Punkt bei $(T, \mu_0) \approx (0.608, 0.318)$

possible QCD-phase diagram



- crystalline LOFF phase (color superconductive phase)?
- problem: $\mu \neq 0 \Rightarrow$ complex fermion determinant ☹
- large μ beyond reach in simulations
- are there inhomogeneous crystallic phases in model systems?

- discrete ε_n energies of Dirac Hamiltonian on $[0, L]$

$$h_\sigma = \gamma^0\gamma^1\partial_x + \gamma^0\sigma(x)$$

- hidden supersymmetry

$$h_\sigma^2 = -\frac{d^2}{dx^2} + \sigma^2(x) - \gamma^1\sigma'(x) = \begin{pmatrix} AA^\dagger & 0 \\ 0 & A^\dagger A \end{pmatrix}, \quad A = -\frac{d}{dx} + \sigma$$

- renormalization: fix (constant) condensate σ_0 at $\mu = T = 0$
- introduce constant companion field

$$\bar{\sigma}^2 = \frac{1}{L}\int dx\,\sigma^2(x)$$

- constant $\sigma \Rightarrow \bar{\sigma} = \sigma$

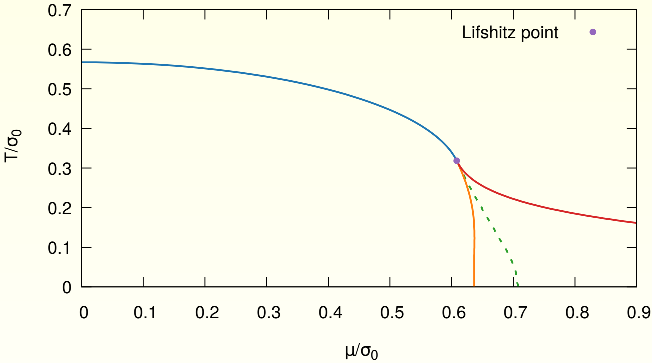
- renormalized effective action for $\sigma = \sigma(x)$

$$S_{\rm eff}[\sigma] = \frac{\beta L}{4\pi}\,\bar\sigma^{\,2}\Big(\log\frac{\bar\sigma^{\,2}}{\sigma_0^2} - 1\Big) + \beta\Big(\sum_{n:\varepsilon_n<0}\varepsilon_n - \sum_{n:\bar\varepsilon_n<0}\bar\varepsilon_n\Big)$$
$$- \sum_{n:\varepsilon_n>0}\Big(\log\big(1+\mathrm{e}^{-\beta(\varepsilon_n+\mu)}\big) + \log\big(1+\mathrm{e}^{-\beta(\varepsilon_n-\mu)}\big)\Big)$$

derive gap equation for inhomogeneous field

$$\frac{\delta S_{\rm eff}}{\delta\sigma(x)} = \frac{1}{2\pi}\sigma(x)\log\frac{\bar\sigma^2}{\sigma_0^2} + \sum_{n:\varepsilon_n<0}\psi_n^\dagger\gamma^0\psi_n - \frac{\sigma(x)}{\bar\sigma}\sum_{n:\bar\varepsilon_n<0}\bar\psi_n^\dagger\gamma^0\bar\psi_n$$
$$+ \sum_{n:\varepsilon_n>0}\left(\frac{1}{1+e^{\beta(\varepsilon_n+\mu)}} + \frac{1}{1+e^{\beta(\varepsilon_n-\mu)}}\right)\psi_n^\dagger\gamma^0\psi_n = 0$$

- solution in terms of elliptic functions $\Rightarrow$ crystal of baryons at large μ, low T

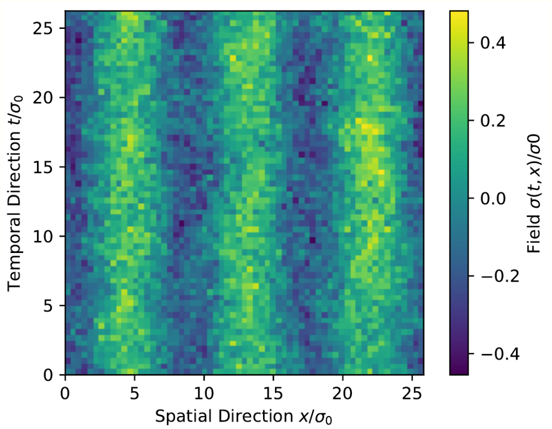


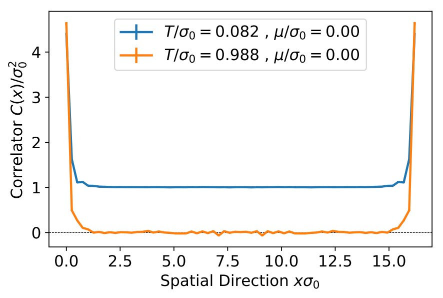
- inhomogeneous condensate for small T, large μ
  $\Rightarrow$ breaking of translation invariance ($\mathrm{N_f} \to \infty$)
- wave-length of condensate $\Leftrightarrow \mu$
- all phase transitions are second order
- cp. Peierls-Fröhlich model, ferromagnetic superconductors

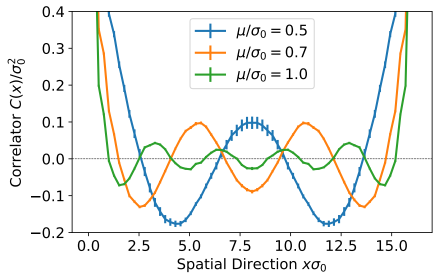
- inhomogeneous $\langle\bar{\psi}\psi\rangle$ breaks translation invariance $\to$ massless Goldstone-excitations $\to$ should not exist in $d = 1 + 1$
- no-go theorems not valid for $\mathrm{N_f} \to \infty$
- phase diagram = artifact of $\mathrm{N_f} \to \infty$?
- is there a inhomogeneous condensate for $\mathrm{N_f} < \infty$?
- number of massless Goldstone excitations:
  n_k number of type k Goldstone modes
  type 1: $\omega \sim |\boldsymbol{k}|^{2n+1}$, e.g. relativistic dispersion relation
  type 2: $\omega \sim |\boldsymbol{k}|^{2n}$, e.g. non-relativistic dispersion relation
  inner symmetries $n_1 + 2n_2 =$number of broken directions
  spacetime symmetries $n_1 + 2n_2 \leq$ number of broken directions
- large μ: dispersion relation need not be relativistic

- update with (nonlocal) determinant of huge matrix D
- potential sign-problem for finite μ
- can prove: fermion determinant is indeed real
  $\Rightarrow$ no sign problem for even $\mathrm{N_f}$
- hybrid MC algorithm, pseudo fermions
- rational approximation of inverse fermion matrix
- simulations with chiral fermions only
  naive fermions for $\mathrm{N_f} = 8, 16$ ($\rightarrow$ doublers)
  simulations with SLAC fermions for $\mathrm{N_f} = 2, 8, 16$
  action of pseudo-fermion field with parallized Fourier transformation
- scale setting: condensate σ_0 at $T = \mu = 0$
- simulations on large lattices $N_s \leq 1024$

- low temperature $T = 0.038\,\sigma_0$, medium density $\mu = 0.5\sigma_0$
- typical configuration for $\mathrm{N_f} = 8$ and $L = 64$







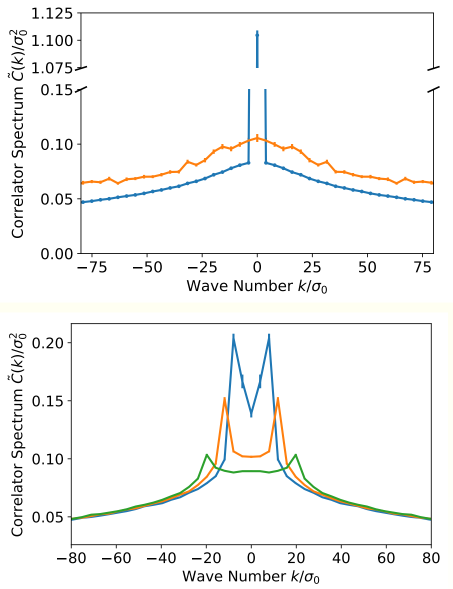
spatial correlation function of chiral condensate

$$C(x) = \frac{1}{L}\sum_y \langle \sigma(y,t)\sigma(y+x,t)\rangle$$

- $\mathrm{N_f} = 8, L = 64$
  naive fermions
- top: homogeneous phase

  $\mu = 0$
  $T/\sigma_0 \in \{0.082, 0.988\}$
- bottom: inhomogeneous phase

  $T = 0.082\sigma_0$
  $\mu/\sigma_0 \in \{0.5, 0.7, 1.0\}$



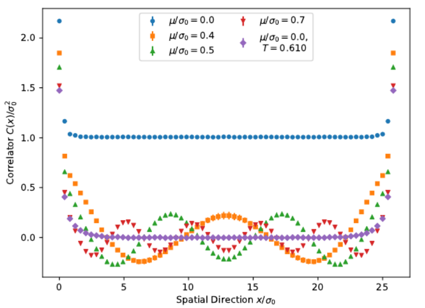
Fourier transform of the spatial correlation function

$$\tilde{C}(k) \propto \sum_x \mathrm{e}^{\mathrm{i}kx} C(x)$$

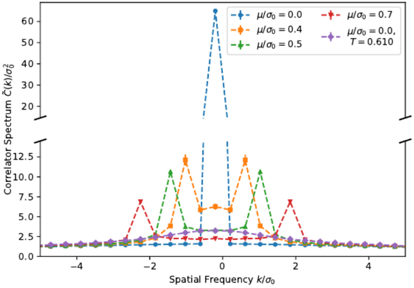
- $\mathrm{N_f} = 8, L = 64$
  naive fermions
- top: homogeneous phases

  $\mu = 0$
  $T/\sigma_0 \in \{0.082, 0.988\}$
- bottom: inhomogeneous phase

  $T = 0.082\,\sigma_0$
  $\mu/\sigma_0 \in \{0.5, 0.7, 1.0\}$

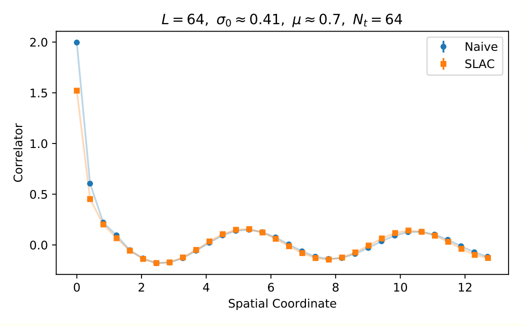


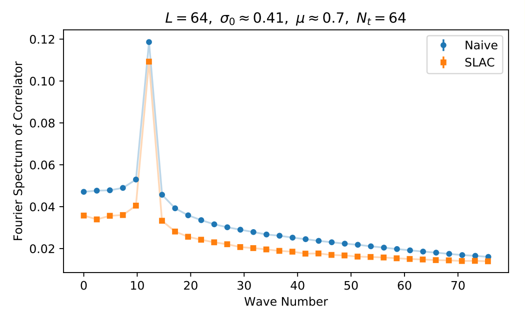
(a) Real space.



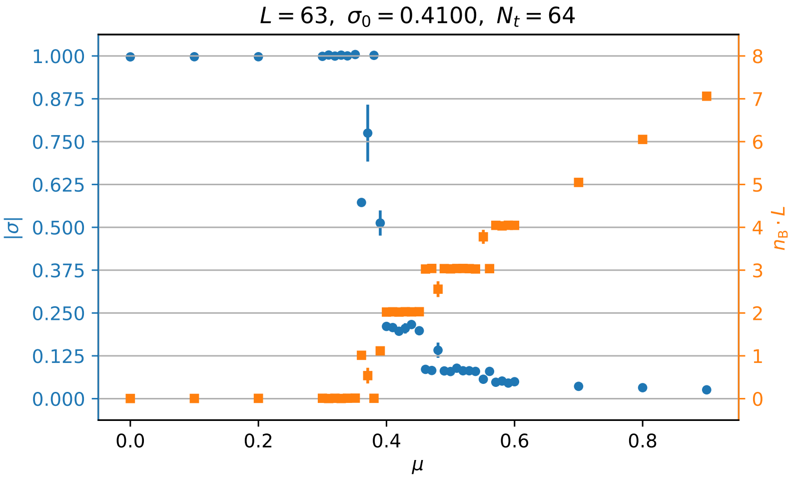
spatial correlation function and Fourier-transform

- $\mathrm{N_f} = 8$, $L = 64$
  SLAC-fermions
- low temperature $T = 0.038\sigma_0$
- different chemical potentials
  $\mu/\sigma_0 \in \{0, 0.4, 0.5, 0.7\}$
- violet:
  symmetric phase
  $\mu = 0, \;\; T = 0.61\,\sigma_0$

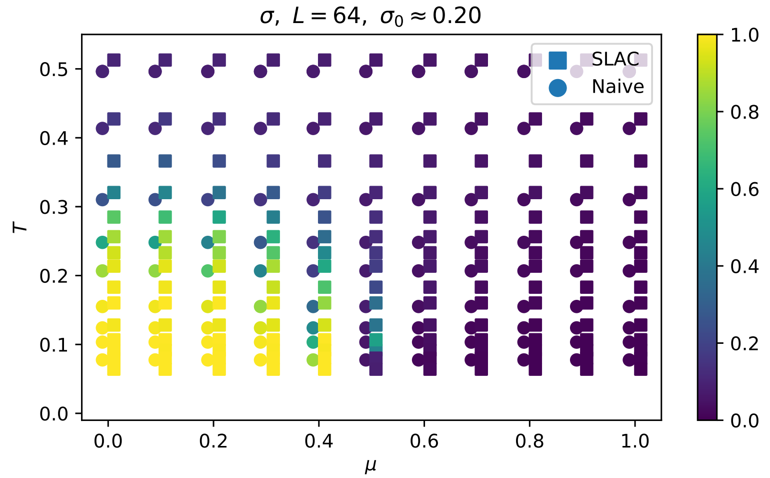


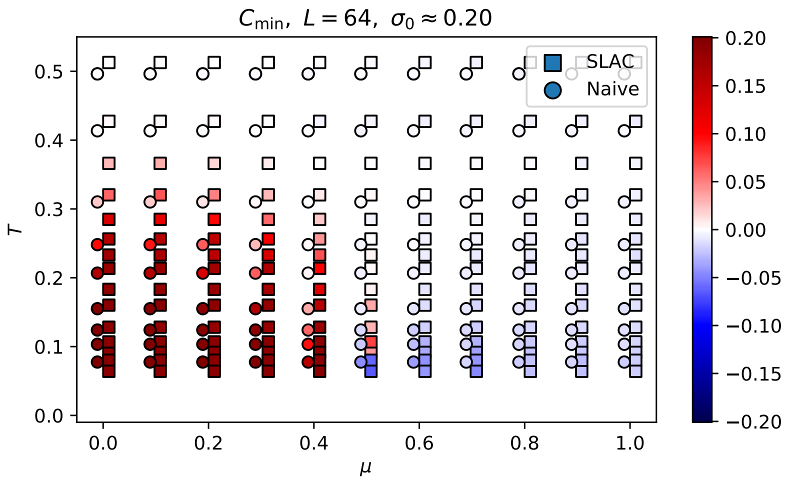


- $N_f = 8$
- crystalline phase
- spatial correlation function for naive and SLAC fermions
- Fourier transform



$L = 63,\ \sigma_0 = 0.4100,\ N_t = 64$
$|\sigma|$
1.000
0.875
0.750
0.625
0.500
0.375
0.250
0.125
0.000
0.0
0.2
0.4
0.6
0.8
μ
$n_B \cdot L$
8
7
6
5
4
3
2
1
0


$\sigma,\ L = 64,\ \sigma_0 \approx 0.20$
SLAC
Naive
T
μ
0.0
0.1
0.2
0.3
0.4
0.5
0.0
0.2
0.4
0.6
0.8
1.0
0.0
0.2
0.4
0.6
0.8
1.0



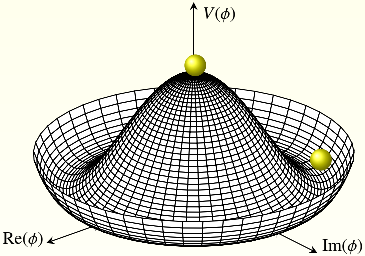
$C_{\min}$, $L = 64$, $\sigma_0 \approx 0.20$
SLAC
Naive
T
μ
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.8
1.0
0.20
0.15
0.10
0.05
0.00
−0.05
−0.10
−0.15
−0.20

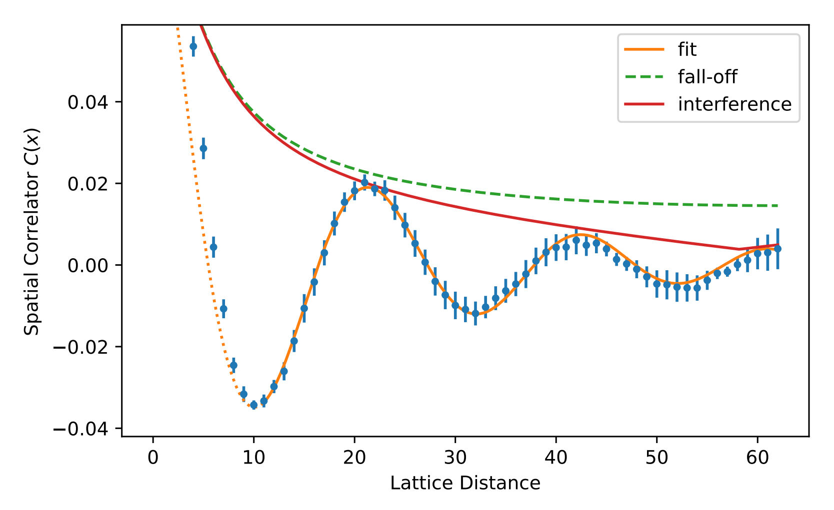
- correlations function for $\mathrm{N_f} \gg 1$

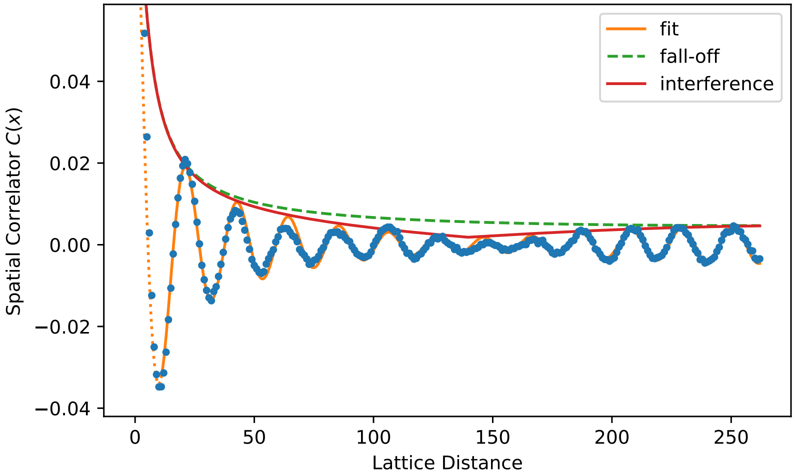
Witten

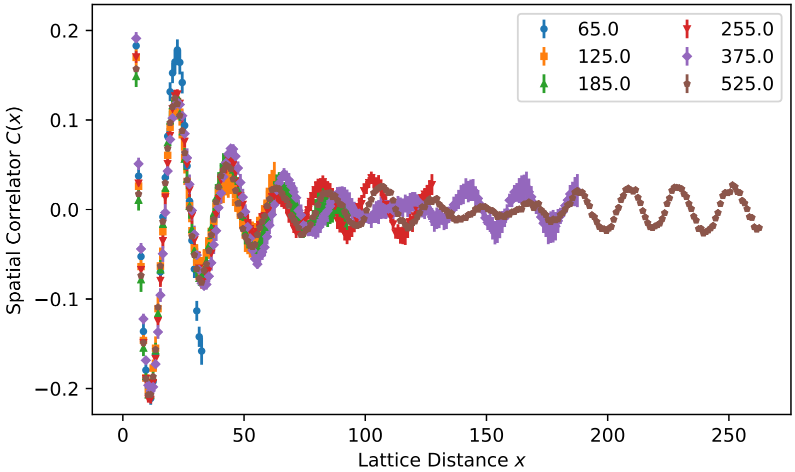
$$C(x, y) \sim \frac{1}{|x-y|^{1/\mathrm{N_f}}}$$

- may look like SSB for large $\mathrm{N_f}$ on small lattices
- dependence on system size
- smallest available $\mathrm{N_f} = 2$
- check algorithmic aspects (e.g. thermalization)




fit
fall-off
interference
Spatial Correlator $C(x)$
Lattice Distance
0.04
0.02
0.00
−0.02
−0.04
0
10
20
30
40
50
60


fit
fall-off
interference
0.04
0.02
0.00
−0.02
−0.04
Spatial Correlator $C(x)$
0
50
100
150
200
250
Lattice Distance


Spatial Correlator $C(x)$
Lattice Distance x
0.2
0.1
0.0
−0.1
−0.2
0
50
100
150
200
250
65.0
125.0
185.0
255.0
375.0
525.0

- first simulation for GN model at finite $\mu, T, \mathrm{N_f}$
- no sign problem for even $\mathrm{N_f}$
- comparable results for $\mathrm{N_f} = 8$ and $\mathrm{N_f} = 16$
  naive and chiral SLAC fermions
- phase diagrams are similar as for $\mathrm{N_f} \to \infty$ Thies
  wave length and amplitude of condensate
- simulations for $\mathrm{N_f} = 2$ on sizable lattices
- Goldstone-theorem, ...
- situation in higher dimensions
- domain walls, vortices, ... ???

Lenz, Pannullo, Wagner, Wellegehausen, AW

- asymptotically safe ($1/\mathrm{N_f}$ expansion, FRG)
- GN model show 2nd order phase transition for all $\mathrm{N_f}$
- $\mathrm{N_f}$ odd: parity breaking
- Thirring models:
  even $\mathrm{N_f}$: no phase transition
  odd $\mathrm{N_f}$: phase transition for $\mathrm{N_f} \leq \mathrm{N_f}^{\mathrm{crit}}$
- critical $\mathrm{N_f}^{\mathrm{crit}}$ determined
- spectrum of light (would be Goldstone) particles
- average spectral density of Dirac operator
- full phase diagram in $(\lambda, \mathrm{N_f})$-plane

B. Wellegehausen, D. Schmidt, AW, Phys.Rev. D96 (2017) 094504

J. Lenz, AW, B. Wellegehausen, arXiv:1905.00137