The Schwinger model in the canonical formulation

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Motivation for the canonical formulation

• Consider the grand-canonical partition function at finite μ :

$$Z_{\mathsf{GC}}(\mu) = \mathsf{Tr}\left[e^{-\mathcal{H}(\mu)/\mathcal{T}}\right] = \mathsf{Tr}\prod_{t}\mathcal{T}_{t}(\mu)$$

- The sign problem at finite density is a manifestation of huge cancellations between different states:
 - all states are present for any μ and ${\it T}$
 - some states need to cancel out at different μ and ${\it T}$
- In the canonical formulation:

$$Z_{\mathsf{C}}(N_f) = \mathsf{Tr}_{N_f}\left[e^{-\mathcal{H}/\mathcal{T}}\right] = \mathsf{Tr}\prod_t \mathcal{T}_t^{(N_f)}$$

- dimension of Fock space tremendously reduced
- Iess cancellations necessary:

• e.g.
$$Z_{C}^{QCD}(N_Q) = 0$$
 for $N_Q \neq 0 \mod N_c$

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 for $N_Q \neq 0$

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- e.g. "Silver Blaze" phenomenon realised automatically

Motivation for canonical formulation of QCD

Canonical transfer matrices can be obtained explicitly!

 based on the dimensional reduction of the QCD fermion determinant [Alexandru, Wenger '10; Nagata, Nakamura '10]

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Outline:

- Overview
- Definition of the transfer matrices in canonical formulation
- Relation to fermion loop and worldline formulations
- Hubbard model and Super Yang-Mills QM
- Schwinger model

Overview

- Identification of transfer matrices:
 - Dimensional reduction in QCD [Alexandru, UW '10]
 - SUSY QM and SUSY Yang-Mills QM [Baumgartner, Steinhauer, UW '12-'15]
 - solution of the sign problem
 - connection with fermion loop formulation
 - QCD in the heavy-dense limit
 - absence of the sign problem at strong coupling
 - solution of the sign problem in the 3-state Potts model [Alexandru, Bergner, Schaich, UW '18]
 - Hubbard model [Burri, UW '19]
 - HS field can be integrated out analytically
 - ► N_f = 1,2 Schwinger model [Bühlmann, UW '19]

General construction

• For a generic Hamiltonian $\mathcal H$ with $\mu \equiv \{\mu_\sigma\}$ one has

$$Z_{GC}(\mu) = \operatorname{Tr}\left[e^{-\mathcal{H}(\mu)/T}\right]$$
$$= \sum_{\{N_{\sigma}\}} e^{-\sum_{\sigma} N_{\sigma} \mu_{\sigma}/T} \cdot Z_{C}(\{N_{\sigma}\})$$

where $Z_C(\{N_{\sigma}\}) = \operatorname{Tr} \prod_t \mathcal{T}_t^{(\{N_{\sigma}\})}$.

Trotter decomposition and coherent state representation yields

$$Z_{\rm GC}(\mu) = \int \mathcal{D}\phi e^{-S_b[\phi]} \int \mathcal{D}\psi^{\dagger} \mathcal{D}\psi e^{-S[\psi^{\dagger},\psi,\phi;\mu]}$$

with Euclidean action S_b and fermion matrix M

$$S[\psi^{\dagger},\psi,\phi;\mu] = \sum_{\sigma} \psi_{\sigma}^{\dagger} M[\phi;\mu] \psi_{\sigma}.$$

Fermion matrix and dimensional reduction

- The fermion matrix $M[\phi; \mu_{\sigma}]$ has the generic structure

$$M = \begin{pmatrix} B_0 & e^{-\mu_{\sigma}} C'_0 & 0 & \dots & \pm e^{\mu_{\sigma}} C_{N_t-1} \\ e^{\mu_{\sigma}} C_0 & B_1 & e^{-\mu_{\sigma}} C'_1 & 0 \\ 0 & e^{\mu_{\sigma}} C_1 & B_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & & \\ & & & B_{N_t-2} & e^{-\mu_{\sigma}} C'_{N_t-2} \\ \pm e^{-\mu_{\sigma}} C'_{N_t-1} & 0 & & e^{\mu_{\sigma}} C_{N_t-2} & B_{N_t-1} \end{pmatrix}$$

for which the determinant can be reduced to

$$\det M[\phi; \mu_{\sigma}] = \prod_{t} \det \tilde{B}_{t} \cdot \det \left(1 \mp e^{N_{t}\mu_{\sigma}} \mathcal{T}[\phi]\right)$$

where $\mathcal{T}[\phi] = \mathcal{T}_{N_{t}-1} \cdot \ldots \cdot \mathcal{T}_{0}$.

• $M[\phi; \mu_{\sigma}]$ is $(L_s \cdot N_t) \times (L_s \cdot N_t)$, while $\mathcal{T}[\phi]$ is $L_s \times L_s$.

Fermion matrix and canonical determinants

Fugacity expansion

$$\det M[\phi; \mu_{\sigma}] = \sum_{N_{\sigma}} e^{-N_{\sigma}\mu_{\sigma}/T} \cdot \det_{N_{\sigma}} M[\phi]$$

yields the canonical determinants

$$\det_{N_{\sigma}} M[\phi] = \sum_{J} \det \mathcal{T}^{\mathsf{X}}[\phi] = \mathsf{Tr}\left[\prod_{t} \mathcal{T}^{(N_{\sigma})}_{t}\right].$$

where det $\mathcal{T}^{\chi\chi}$ is the principal minor of order N_{σ} .

- States are labeled by index sets $J \subset \{1, \dots, L_s\}, |J| = N_\sigma$
 - number of states grows exponentially with L_s at half-filling

$$N_{\text{states}} = \begin{pmatrix} L_s \\ N_\sigma \end{pmatrix} = N_{\text{principal minors}}$$

sum can be evaluated stochastically with MC

Transfer matrices

Use Cauchy-Binet formula

$$\det(A \cdot B)^{\lambda \not k} = \sum_{J} \det A^{\lambda \not k} \cdot \det B^{\lambda \not k}$$

to factorize into product of transfer matrices

• Transfer matrices in sector N_σ are hence given by

$$(\mathcal{T}_t^{(N_\sigma)})_{IK} = \det \tilde{B}_t \cdot \det [\mathcal{T}_t]^{kk}$$

with $\operatorname{Tr}\left[\prod_{t} \mathcal{T}_{t}^{(N_{\sigma})}\right] = (\mathcal{T}_{N_{t}-1}^{(N_{\sigma})})_{IJ} \cdot (\mathcal{T}_{N_{t}-2}^{(N_{\sigma})})_{JK} \cdot \ldots \cdot (\mathcal{T}_{0}^{(N_{\sigma})})_{LI}.$

Finally, we have

$$Z_{\mathcal{C}}(\{N_{\sigma}\}) = \int \mathcal{D}\phi \, e^{-S_{b}[\phi]} \prod_{t} \det \tilde{B}_{t} \cdot \sum_{\{J_{t}^{\sigma}\}} \prod_{t} \left(\prod_{\sigma} \det \left[\mathcal{T}_{t}^{\sigma}\right]^{\mathcal{X}_{t-1}^{\sigma} \mathcal{X}_{t}^{\sigma}} \right)$$

where $|J_t^{\sigma}| = N_{\sigma}$ and $J_{N_t}^{\sigma} = J_0^{\sigma}$.

· Consider the Hamiltonian for the Hubbard model

$$\mathcal{H}(\mu) = -\sum_{\langle x, y \rangle, \sigma} t_{\sigma} \, \hat{c}_{x, \sigma}^{\dagger} \hat{c}_{y, \sigma} + \sum_{x, \sigma} \mu_{\sigma} N_{x, \sigma} + U \sum_{x} N_{x, \uparrow} N_{x, \downarrow}$$

with particle number $N_{x,\sigma} = \hat{c}_{x,\sigma}^{\dagger} \hat{c}_{x,\sigma}$.

 After Trotter decomposition and Hubbard-Stratonovich transformation we have

$$Z_{\mathsf{GC}}(\mu) = \int \mathcal{D}\psi^{\dagger} \mathcal{D}\psi \mathcal{D}\phi \rho[\phi] e^{-\sum_{\sigma} S[\psi_{\sigma}^{\dagger}, \psi_{\sigma}, \phi; \mu_{\sigma}]}$$

with $S[\psi_{\sigma}^{\dagger}, \psi_{\sigma}, \phi; \mu_{\sigma}] = \psi_{\sigma}^{\dagger} M[\phi; \mu_{\sigma}] \psi_{\sigma}$, and hence

$$= \int \mathcal{D}\phi \,\rho[\phi] \prod_{\sigma} \det M[\phi;\mu_{\sigma}] \,.$$

The fermion matrix has the structure

$$M[\phi; \mu_{\sigma}] = \begin{pmatrix} B & 0 & \dots & \pm e^{\mu_{\sigma}} C(\phi_{N_{t}-1}) \\ -e^{\mu_{\sigma}} C(\phi_{0}) & B & \dots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \dots & -e^{\mu_{\sigma}} C(\phi_{N_{t}-2}) & B \end{pmatrix}$$

for which the determinant can be reduced to

$$\det M[\phi; \mu_{\sigma}] = \det B^{N_t} \cdot \det \left(1 \mp e^{N_t \mu_{\sigma}} \mathcal{T}[\phi]\right)$$

where $\mathcal{T}[\phi] = B^{-1}C(\phi_{N_t-1})\cdot\ldots\cdot B^{-1}C(\phi_0).$

Fugacity expansion yields the canonical determinants

$$\det M_{N_{\sigma}}[\phi] = \sum_{J} \det \mathcal{T}^{\mathfrak{U}}[\phi] = \operatorname{Tr}\left[\prod_{t} \mathcal{T}_{t}^{(N_{\sigma})}\right].$$

where det $\mathcal{T}^{\chi\chi}$ is the principal minor of order N_{σ} .

Transfer matrices are hence given by

$$(\mathcal{T}_t)_{IK} = \det B \cdot \det \left[B^{-1} \cdot C(\phi_t) \right]^{NK}$$
$$= \det B \cdot \det(B^{-1})^{N} \cdot \det C(\phi_t)^{NK}$$

Moreover, using the complementary cofactor we get

$$\det B \cdot \det(B^{-1})^{\mathcal{Y}} = (-1)^{p(I,J)} \det B^{IJ}$$

where $p(I, J) = \sum_{i} (I_i + J_i)$ and HS field can be integrated out,

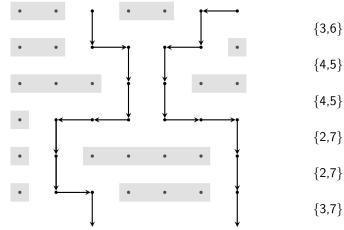
$$\det C(\phi_t)^{\mathcal{Y}_{K}} = \delta_{JK} \prod_{x \notin J} \phi_{x,t} \implies \prod_{x} w_{x,t} \equiv W(\{J_t^{\sigma}\}).$$

Finally, only sum over discrete index sets is left:

$$Z_{C}(\{N_{\sigma}\}) = \sum_{\{J_{\tau}^{\sigma}\}} \prod_{t} \left(\prod_{\sigma} \det B^{J_{\tau-1}^{\sigma}J_{\tau}^{\sigma}} \right) W(\{J_{t}^{\sigma}\}), \quad |J_{t}^{\sigma}| = N_{\sigma}$$

$$Z_{C}(\{N_{\sigma}\}) = \sum_{\{J_{t}^{\sigma}\}} \prod_{t} \left(\prod_{\sigma} \det B^{J_{t-1}^{\sigma}J_{t}^{\sigma}}\right) W(\{J_{t}^{\sigma}\})$$

index sets J_t :



In d = 1 dimension the 'fermion bags' det B^{IJ} can be calculated analytically:

and one can prove that

det $B^{IJ} \ge 0$ for open b.c.

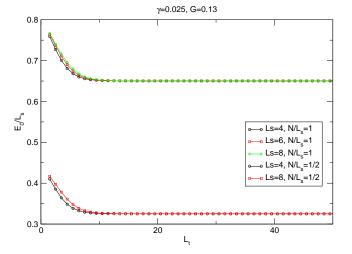
 \Rightarrow there is no sign problem

• For periodic b.c. there is no sign problem either, because

$$Z_C^{\rm pbc}(L_s \to \infty) = Z_C^{\rm obc}(L_s \to \infty)$$

Since our formulation is factorized in time, we have

$$E_0 = \lim_{L_t \to \infty} \frac{Z_C(L_t)}{Z_C(L_{t+1})} = \left\langle \prod_{\sigma} \left(\frac{\det B^{J_{t-1}^{\sigma} J_{t+1}^{\sigma}}}{\det B^{J_{t-1}^{\sigma} J_t^{\sigma}} \det B^{J_t^{\sigma} J_{t+1}^{\sigma}}} \right) \frac{1}{W(\{J_t^{\sigma}\})} \right\rangle_{Z_C(L_{t+1})}$$



Grand canonical gauge theories

Consider gauge theory, e.g. Schwinger model or QCD:

$$Z_{\mathsf{GC}}(\mu) = \int \mathcal{D}U \mathcal{D}\overline{\psi} \mathcal{D}\psi \, e^{-S_g[U] - S_f[\overline{\psi}, \psi, U; \mu]}$$

where

$$\begin{split} S_g[U] &= \beta \sum_P \left[1 - \frac{1}{2} \left(U_P + U_P^{\dagger} \right) \right], \\ S_f[\overline{\psi}, \psi, U; \mu] &= \overline{\psi} M[U; \mu] \psi \,. \end{split}$$

- for QCD: $d = 4, U \in SU(N_c)$
- for the Schwinger model: $d = 2, U \in U(1)$
- Integrating out the Grassmann fields for N_f flavours yields

$$Z_{\mathsf{GC}}(\mu) = \int \mathcal{D}U \, e^{-S_{g}[U]} \, (\det M[U;\mu])^{N_{f}}$$

Dimensional reduction of gauge theories

 Consider the Wilson fermion matrix for a single quark with chemical potential µ:

- B_t are (spatial) Wilson Dirac operators on time-slice t,
- Dirac projectors $P_{\pm} = \frac{1}{2}(\mathbb{I} \mp \Gamma_4)$,
- temporal hoppings are

$$A_t^+ = e^{+\mu} \cdot \mathbb{I}_{d \times d} \otimes \mathcal{U}_t = (A_t^-)^{-1}$$

• all blocks are $(d \cdot N_c \cdot L_s^3 \times d \cdot N_c \cdot L_s^3)$ -matrices

Dimensional reduction of gauge theories

Reduced Wilson fermion determinant is given by

$$\det M_{p,a}(\mu) = \prod_{t} \det Q_{t}^{+} \cdot \det \left[\mathbb{I} \pm e^{+\mu L_{t}} \mathcal{T} \right]$$

where $\ensuremath{\mathcal{T}}$ is a product of transfer matrices given by

$$\mathcal{T} = \prod_{t} \mathcal{U}_{t-1}^{+} \cdot \left(\mathcal{Q}_{t}^{-} \right)^{-1} \cdot \mathcal{Q}_{t}^{+} \cdot \mathcal{U}_{t}^{-}$$

with

$$Q_t^{\pm} = B_t P_{\pm} + P_{\mp}, \qquad \mathcal{U}_t^{\pm} = \mathcal{U}_t P_{\pm} + P_{\mp}$$

• Fugacity expansion yields with $N_Q^{\text{max}} = d \cdot N_c \cdot L_s^3$

$$\det M_a(\mu) = \sum_{N_Q = -N_Q^{\max}}^{N_Q^{\max}} e^{\mu N_Q/T} \cdot \det M_{N_Q}$$

Canonical transfer matrices of gauge theories

$$\det M_{N_Q} = \prod_t \det Q_t^+ \cdot \sum_A \det \mathcal{T}^{\lambda_t \lambda_t} = \operatorname{Tr} \prod_t \mathcal{T}_t^{(N_Q)}$$

- sum is over all index sets $A \in \{1, 2, \dots, 2N_Q^{\max}\}$ of size N_Q ,
- i.e. the trace over the minor matrix of rank N_Q of \mathcal{T}

 Provides a complete temporal factorization of the fermion determinant.

Relation between quark and baryon number in QCD

• Consider $\mathbb{Z}(N_c)$ -transformation by $z_k = e^{2\pi i \cdot k/N_c} \in \mathbb{Z}(N_c)$:

$$U_4(x) \rightarrow U_4(x)' = (1 + \delta_{x_4,t} \cdot (\mathbf{z}_k - 1)) \cdot U_4(x)$$

- Hence, \mathcal{U}_{x_4} transforms as $\mathcal{U}_{x_4} \to \mathcal{U}'_{x_4} = \underline{z_k} \cdot \mathcal{U}_{x_4}$, while for all others $\mathcal{U}'_{t\neq x_4} = \mathcal{U}_{t\neq x_4}$.
- As a consequence we have

$$\det M_{N_Q} \to \det M'_{N_Q} = \prod_t \det Q_t^+ \cdot \sum_A \det(\underline{z_k} \cdot \mathcal{T})^{\lambda_{k_q}}$$
$$= \underline{z_k^{-N_Q}} \cdot \det M_{N_Q}$$

and summing over z_k therefore yields

 $\det M_{N_Q} = 0 \qquad \text{for } N_Q \neq 0 \mod N_c$

• reduces cancellations by factor of N_c

Gauss' law in the $N_f = 1$ Schwinger model

• Consider U(1)-transformation by $e^{i\alpha} \in U(1)$:

$$e^{i\phi_2(x)} \rightarrow e^{i\phi_2(x)\prime} = \left(1 + \delta_{x_2,t} \cdot \left(e^{i\alpha} - 1\right)\right) \cdot e^{i\phi_2(x)}$$

- Hence, \mathcal{U}_{x_2} transforms as $\mathcal{U}_{x_2} \rightarrow \mathcal{U}'_{x_2} = e^{i\alpha} \cdot \mathcal{U}_{x_2}$, while for all others $\mathcal{U}'_{t\neq x_2} = \mathcal{U}_{t\neq x_2}$.
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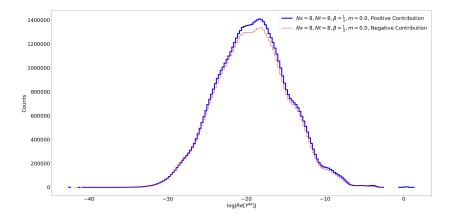
$$\det M_{N_Q} \to \det M'_{N_Q} = \prod_t \det Q_t^+ \cdot \sum_A \det(e^{i\alpha} \cdot \mathcal{T})^{\lambda_{A_Q}}$$
$$= e^{-i\alpha N_Q} \cdot \det M_{N_Q}$$

and integrating over α therefore yields

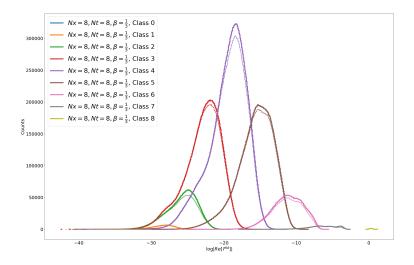
$$\det M_{N_Q} = 0 \qquad \text{for } N_Q \neq 0$$

only zero charge sector is allowed!

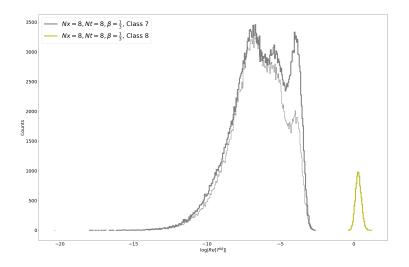
• Distribution of principal minors:



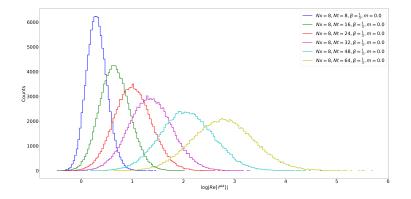
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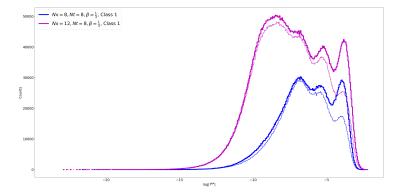
Distribution of maximal principal minors:



• Distribution of maximal principal minors (ground state):



• Distribution of next-to-maximal principal minors (exc. states):



- Physics in the 2-flavour model is more interesting,
 - denote the fermion flavours by u and d.
- Isospin chemical potential generates multi-meson states.
- Number of *u* and *d*-fermions must be equal:

charge $Q = n_u + n_d = 0 \iff$ Gauss' law, isospin $I = (n_u - n_d)/2$ arbitrary

• Corresponding canonical partition functions (with $n_u = -n_d$):

$$Z_{n_u,n_d} = \int \mathcal{D}\phi \, e^{-S_g[\phi]} \det_{n_u} M_u[\phi] \det_{n_d} M_d[\phi].$$

• Vacuum sector is described by $Z_{0,0}$.

Calculating the pion energy

- The flavour-triplet meson (pion) $|\overline{\psi}\gamma_5\tau^a\psi\rangle$ has quantum numbers

$$Q = 0$$
 fermion number
 $I = 1$ isospin

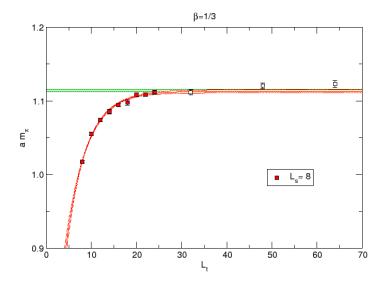
and is the groundstate of the system with $n_u = +1$, $n_d = -1$:

$$Z_{+1,-1} = \int \mathcal{D}\phi \, e^{-S_g[\phi]} \det_{+1} M_u[\phi] \det_{-1} M_d[\phi].$$

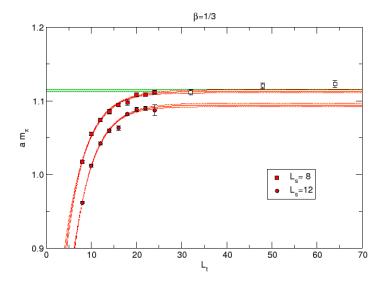
• The free energy difference to the vacuum at $T \rightarrow 0$ defines the pion mass:

$$m_{\pi}(L) = -\lim_{L_t \to \infty} \frac{1}{L_t} \log \frac{Z_{+1,-1}(L_t)}{Z_{0,0}(L_t)} \equiv \mu_1(L)$$

Calculating the pion energy



Calculating the pion energy



Calculating the 2-pion energy

• The flavour-triplet 2-meson (pion) state $|\pi\pi\rangle$ has quantum numbers

Q = 0 fermion number I = 2 isospin

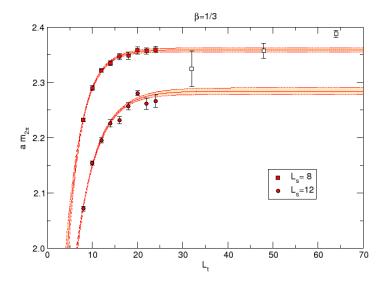
and is the groundstate of the system with $n_u = +2$, $n_d = -2$:

$$Z_{+2,-2} = \int \mathcal{D}\phi \, e^{-S_g[\phi]} \det_{+2} M_u[\phi] \det_{-2} M_d[\phi].$$

The free energy difference to the vacuum at T → 0 defines the energy of the 2-pion system:

$$E_{2\pi}(L) = -\lim_{L_t \to \infty} \frac{1}{L_t} \log \frac{Z_{+2,-2}(L_t)}{Z_{0,0}(L_t)} \equiv \mu_1(L) + \mu_2(L)$$

Calculating the 2-pion energy



Scattering phase shifts

• $m_{\pi}(L)$ and $E_{2\pi}(L)$ can be described by 3 parameters:

$$m_{\pi}(L) = m_{\infty} + Ae^{-m_{\infty}L}/\sqrt{L}$$

 $E_{2\pi}(L) = 2\sqrt{m_{\pi}(L)^2 + p^2}$

where p is determined through the scattering phase shift

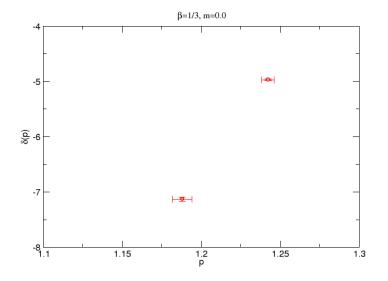
$$\delta(p) = -\frac{pL}{2}$$
, or rather $\delta(p(L)) = -\frac{p(L)L}{2} \equiv \delta(L)$.

From this one can predict the 3-pion energy

$$E_{3\pi}(L) = \sum_{j=1}^{3} \sqrt{m_{\pi}(L)^2 + p_j^3} \equiv \sum_{i=1}^{3} \mu_i(L)$$

with $p_2 = p_3 = -p_1/2 = -2\delta(L)/L$.

Scattering phase shifts



Summary

- Canonical formulation of field theories:
 - transfer matrices can be obtained explicitly
 - close connection to fermion loop or worldline formulations
 - fermionic degrees of freedom are local occupation numbers $n_x = 0, 1$ (encoded in index sets)

Formalism and techniques are generically applicable:

- sometimes solves (or avoids) the fermion sign problem,
- improved estimators for fermionic correlation functions,
- integrating out (auxiliary) fields in some cases possible:
 - \Rightarrow projection to baryon or zero charge sectors
 - \Rightarrow the HS field in the Hubbard model