The Hubbard model in the canonical formulation

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Motivation for the canonical formulation

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

$$Z_{\mathrm{GC}}(\mu) = \mathrm{Tr}\left[e^{-\mathcal{H}(\mu)/T}\right] = \mathrm{Tr}\prod_t \mathcal{T}_t(\mu)$$

- The sign problem at finite density is a manifestation of huge cancellations between different states:
  - all states are present for any μ and T
  - some states need to cancel out at different μ and T

- In the canonical formulation:

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

  - dimension of Fock space tremendously reduced
  - less cancellations necessary
  - e.g. $Z_{\mathrm{C}}^{\mathrm{QCD}}(N_Q) = 0$ for $N_Q \neq 0 \bmod N_c$

Motivation for the canonical formulation

Canonical transfer matrices can be obtained explicitly!

- Based on the dimensional reduction of the fermion determinant [Alexandru, Wenger '10; Nagata, Nakamura '10]
- Identification of transfer matrices:
  - QCD [Alexandru, Wenger '10]
  - 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, Wenger '18]
  - SUSY QM and SUSY Yang-Mills QM [Baumgartner, Steinhauer, Wenger '12-'15]
    - solution of the sign problem
    - connection with (dual) fermion loop formulation

Motivation for the canonical formulation

- Close connection to
  - (dual) fermion loop or worldline formulation
    $\Rightarrow$ worm algorithm
  - fermion bag approach.
- Moreover,
  - fermionic degrees of freedom are local occupation numbers $n_x = 0, 1$,
  - allows local (multi-level) update schemes,
  - improved estimators for fermionic correlation functions,
  - integrating out auxiliary fields in some cases possible:
    $\Rightarrow$ e.g., the HS field in the Hubbard model

Hamiltonian and partition functions

- Consider the Hamiltonian for the Hubbard model

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

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

- The partition function is

$$\begin{aligned} Z_{\mathrm{GC}}(\mu) &= \mathrm{Tr}\left[e^{-\mathcal{H}(\mu)/T}\right] \\ &= \sum_{\{N_\sigma\}} e^{-\sum_\sigma N_\sigma \mu_\sigma/T}\cdot Z_C(\{N_\sigma\}) \end{aligned}$$

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

Coherent state representation and field theory

- Trotter decomposition and coherent state representation yields

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

with Euclidean action

$$S[\psi^\dagger,\psi;\mu] = \sum_\sigma \psi_\sigma^\dagger \nabla_t \psi_\sigma + H[\psi^\dagger,\psi;\mu]\,.$$

- After a Hubbard-Stratonovich transformation we have

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

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

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

Fermion matrix and dimensional reduction

- 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

$$\det M_{N_\sigma}[\phi] = \sum_J \det \mathcal{T}^{JJ}[\phi] = \mathrm{Tr}\left[\prod_t \mathcal{T}_t^{(N_\sigma)}\right].$$

  where $\det \mathcal{T}^{JJ}$ is the principal minor of order N_σ.

Canonical determinants and transfer matrices

- Canonical determinant:

$$\det M_{N_\sigma}[\phi] = \sum_J \det \mathcal{T}^{JJ}[\phi] = \mathrm{Tr}\left[\prod_t \mathcal{T}_t^{(N_\sigma)}\right]$$

  - states are labeled by index sets

$$J \subset \{1, \ldots, L_s\}, \quad |J| = N_\sigma$$

  - 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

$$\det(A \cdot B)^{\bcancel{I}\bcancel{K}} = \det A^{\bcancel{I}\bcancel{J}} \cdot \det B^{\bcancel{J}\bcancel{K}}$$

to factorize into product of transfer matrices

- Transfer matrices are hence given by

$$\begin{aligned}(\mathcal{T}_t)_{IK} &= \det B \cdot \det \left[B^{-1} \cdot C(\phi_t) \right]^{\bcancel{I}\bcancel{K}} \\ &= \det B \cdot \det(B^{-1})^{\bcancel{I}\bcancel{J}} \cdot \det C(\phi_t)^{\bcancel{J}\bcancel{K}}\end{aligned}$$

- Moreover, using the complementary cofactor we get

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

where $p(I,J) = \sum_i (I_i + J_i)$.

Transfer matrices

- Since $C(\phi_t)$ can be chosen diagonal, we have

$$\det C(\phi_t)^{JK} = \delta_{JK} \prod_{x \notin J} \phi_{x,t}$$

and the HS field can be integrated out site by site:

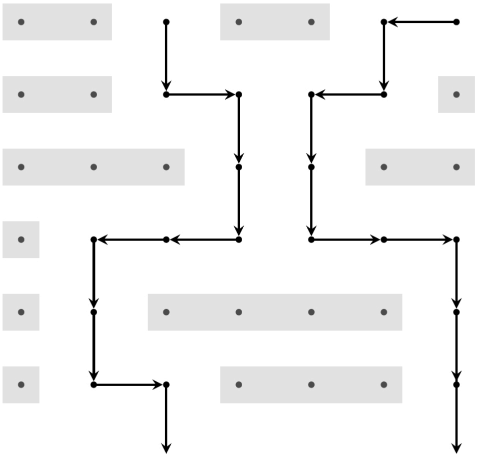
$$\int d\phi_{x,t}\, \rho(\phi_{x,t})\, \phi_{x,t}^{\sum_\sigma \delta_{x \notin J^\sigma}} \equiv w_{x,t} = \begin{cases} w_2 & \text{if } x \notin J^\uparrow, x \notin J^\downarrow \\ w_1 & \text{else} \\ w_0 & \text{if } x \in J^\uparrow, x \in J^\downarrow \end{cases}$$

- Finally, with $\prod_x w_{x,t} \equiv W(\{J_t^\sigma\})$ we have

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

Relation to fermion loop formulation

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



index sets J_t:

{3,6}

{4,5}

{4,5}

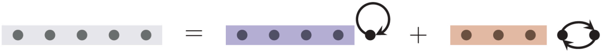
{2,7}

{2,7}

{3,7}

Relation to fermion bag formulation

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



and one can prove that

$$\det B^{IJ} \geq 0 \quad \text{for open b.c.}$$

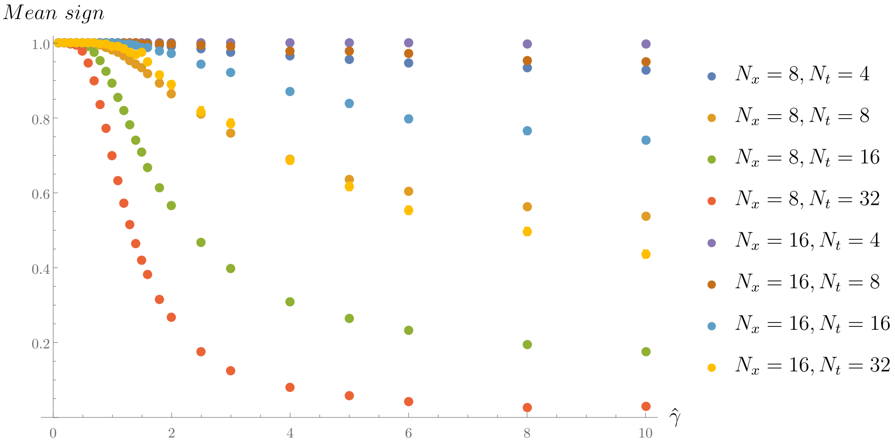
$\Rightarrow$ there is no sign problem

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

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

Sign problem in $d = 1$ dimension

- In the thermodynamic limit $L_s/T \to \infty$ the sign problem is absent for pbc:



The ground state energy

- The energy of the ground state is defined by

$$E_0 = -\lim_{\beta\to\infty} \frac{\partial}{\partial\beta} \ln Z(\beta)$$

and the derivative can be written on the lattice as

$$-\frac{\partial}{\partial\beta} \ln Z(\beta) \to -\frac{\ln Z(L_{t+1}) - \ln Z(L_t)}{\delta t}$$

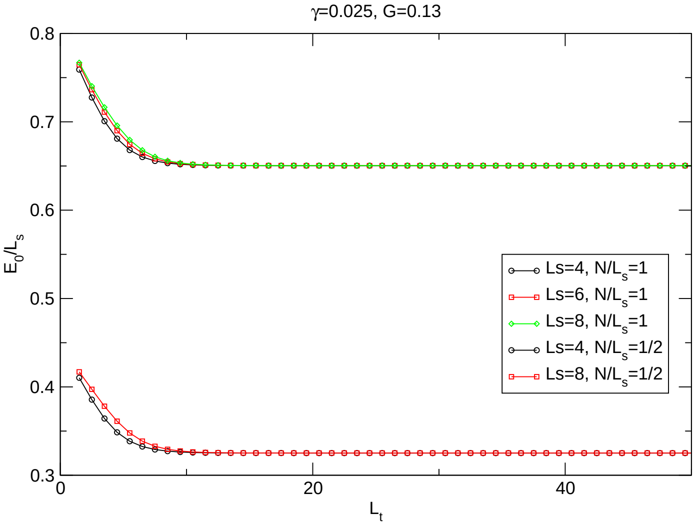
such that

$$E_0 = \lim_{L_t\to\infty} \frac{1}{\delta t} \ln \frac{Z(L_t)}{Z(L_{t+1})}$$

- Since our formulation is factorized in time, we have

$$\frac{Z_C(L_t)}{Z_C(L_{t+1})} = \left\langle \prod_\sigma \left(\frac{\det B^{J^\sigma_{t-1} J^\sigma_{t+1}}}{\det B^{J^\sigma_{t-1} J^\sigma_t} \det B^{J^\sigma_t J^\sigma_{t+1}}} \right) \frac{1}{W(\{J^\sigma_t\})} \right\rangle_{Z_C(L_{t+1})}$$

The ground state energy



Chemical potentials

- The chemical potentials $\mu_{(s)}$ are defined as

$$\mu_{(s)} = \frac{\partial F(n_{(s)})}{\partial n_{(s)}} \quad \text{with } n_{(s)} = N_\uparrow \pm N_\downarrow$$

  which on the lattice can be written as, e.g.,

$$\mu = \frac{F(n+2, n_s) - F(n, n_s)}{2} = -\frac{1}{2\beta} \ln\left(\frac{Z(n+2, n_s)}{Z(n, n_s)}\right)$$

- Now define the partition function for the fermionic 2-pt. fct.

$$Z_t^{\text{2-pt.},\uparrow}(\{N_\sigma\}) = \mathrm{Tr}\left[P^\dagger \prod_{t'<t} \mathcal{T}_{t'}^{\{N_\uparrow+1, N_\downarrow\}} P \cdot \prod_{t'\geq t} \mathcal{T}_{t'}^{\{N_\sigma\}}\right] = \langle\!\langle \psi_0^\dagger \psi_t \rangle\!\rangle_{\{N_\sigma\}}$$

Chemical potentials and telescope product

- then the chemical potential can be expressed

$$e^{-2\mu/T} = \frac{Z(n+2,n_s)}{Z(n,n_s)} = \frac{Z(n+1,n_s+1)}{Z(n,n_s)} \cdot \frac{Z(n+2,n_s)}{Z(n+1,n_s+1)}$$

$$= \frac{Z_0^{\text{2-pt.},\uparrow}}{Z(n,n_s)} \cdot \frac{Z_1^{\text{2-pt.},\uparrow}}{Z_0^{\text{2-pt.},\uparrow}} \cdot \frac{Z_2^{\text{2-pt.},\uparrow}}{Z_1^{\text{2-pt.},\uparrow}} \cdot \ldots \cdot \frac{Z(n+1,n_s+1)}{Z_{Lt-1}^{\text{2-pt.},\uparrow}}$$

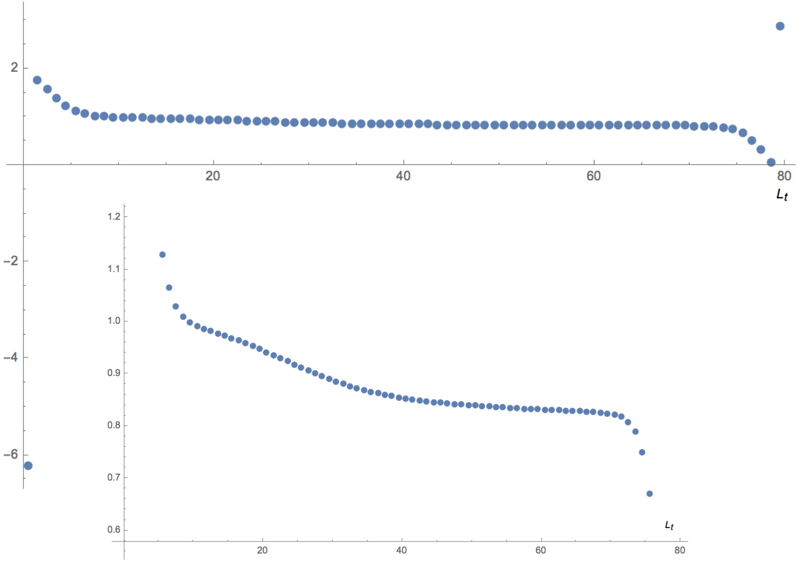
$$\times \frac{Z_0^{\text{2-pt.},\downarrow}}{Z(n+1,n_s+1)} \cdot \frac{Z_1^{\text{2-pt.},\downarrow}}{Z_0^{\text{2-pt.},\downarrow}} \cdot \ldots \cdot \frac{Z(n+2,n_s)}{Z_{L_t-1}^{\text{2-pt.},\downarrow}}$$

where each ratio can be written as an expectation value, e.g.,

$$\frac{Z_{t+1}^{\text{2-pt.},\uparrow}}{Z_t^{\text{2-pt.},\uparrow}} = \left\langle \frac{\sum_{\{J'_{t+1}\}} \det B^{J_t'^{\uparrow} J'_{t+1}} \cdot W(\{J_t'^{\uparrow}, J_t^{\downarrow}\})}{\sum_{\{J_t\}} \det B^{J_t J_{t+1}{}^{\uparrow}} \cdot W(\{J_t, J_t{}^{\downarrow}\})} \right\rangle_{Z_t^{\text{2-pt.},\uparrow}}$$

where $|J'_{t+1}| = |J_t| + 1 = N_\uparrow + 1$.

Chemical potential at $N/L_s = 1/2, L_s = 6, g = 1.0, \gamma = 0.1$



Conclusions

- The Hubbard model

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

in the canonical formulation

$$Z_C(\{N_\sigma\}) = \mathrm{Tr}_{\{N_\sigma\}}\left[e^{-\mathcal{H}/T}\right] = \mathrm{Tr} \prod_t \mathcal{T}_t^{\{(N_\sigma)\}}$$

Canonical transfer matrices can be obtained explicitly!

- Hubbard-Stratonovich field can be integrated out,
- only degrees of freedom are discrete index sets.