O(3) model at nonzero density through matrix product states

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[in progress]
The O(3) model in 2d

\[ S = \frac{1}{2g} \int d^2 x \left( \partial_\nu \vec{n} \right)^2, \quad \vec{n} \in S^2 \]

as an important toy model for 4d QCD:

- asymptotically free = negative $\beta$-function
- dynamical mass generated (although coupling $g$ dimensionless)
- lowest such model of the $O(N)$ and of the $CP(N - 1)$ series
- topology, instantons, theta-angle, renormalons and resurgence
- integrable = infinitely many conserved quantities
- lattice = hoppings in time and space, using $n_1 + in_2 = n_{12}$:

\[ S = -\frac{1}{g} \sum_{x,\nu} \left[ n_3(x)n_3(x + \hat{\nu}) + \frac{1}{2} n_{12}^*(x)n_{12}(x + \hat{\nu}) + \frac{1}{2} n_{12}(x)n_{12}^*(x + \hat{\nu}) \right] \]
nonzero chem. potential for one global $O(2) = U(1)$:

$$n_3(x)n_3(x + \hat{\nu}) + \frac{1}{2} n^*_1 n_2(x + \hat{\nu}) e^{\mu \delta_{\nu,0}} + \frac{1}{2} n^*_2 n_1(x + \hat{\nu}) e^{-\mu \delta_{\nu,0}}$$

action not real $\Rightarrow$ sign problem

exact transformation to dual variables
positive weights $\Rightarrow$ sign problem solved

FB, Kloiber, Gattringer, Sulejmanpasic 14-16
Hamiltonian approach to the O(3) model

Hamilton operator:

- kinetic term of a vector $\vec{n}$ on $S^2 \equiv$ orbital angular momentum
- chemical potential (magnetic field) couples to 3rd component
  $$\hat{H} \sim \hat{J}^2, \mu \hat{J}_z$$

- suggests spherical harmonics $|j, m\rangle$, in which
  $$\hat{H} \to j(j+1), \mu m$$
  no complex numbers in Hamiltonian approach (still hermitian)
  but search for ground state

- O(3) model = 1d angular momentum chain
  O(2)=XY: Yang et al. 15-17
  use these operators and states on each site $x$ separately
potential term = spatial hoppings $\vec{n}_x \vec{n}_{x \pm \hat{1}}$

representation of position vector $\hat{n}$ in $|j, m\rangle$

\[
\langle j, m| \left\{ \hat{n}_{12}^\dagger, \hat{n}_{12}, \hat{n}_3 \right\} |j', m'\rangle \sim \langle j, 0; 1, 0|j'0\rangle \cdot \langle j, -m; 1, \begin{ cases} +1 \\ -1 \end{ cases} 0 |j', m'\rangle
\]

Clebsch-Gordons (real)

few nonzero: iff triangle condition for $j'$'s and conservation of $m$'s

in $\hat{H}$: combine such expressions at $x$ and $x \pm \hat{1}$

technicality: when truncating the Hilbert space in $|j,m\rangle$ later, the normalization of $\hat{n}$ and its commuting algebra are violated mildly
Ground state of the O(3) model

in sector $Q$ at strong coupling

- leading Hamiltonian:

$$\hat{H} \sim \frac{g}{2} \sum_x \hat{J}^2 \rightarrow \frac{g}{2} \sum_x j_x (j_x + 1)$$

angular momentum $j$ suppressed, prefers $(j, m)_x = (0, 0) \forall \text{ sites } x$

- charge $Q = \sum_x \hat{J}_{z,x} \rightarrow \sum_x m_x$ needs $(j, m)_x = (1, 1)$ at $Q$ sites

- effectively qubits: occupation numbers “0” or “1” with Hamiltonian

$$\hat{H} = \frac{g}{2} \sum_x \hat{n}_x (\hat{n}_x + 1) - \frac{1}{g} \sum_x (\hat{a}_x \hat{a}^\dagger_{x+1} + \hat{a}_{x+1} \hat{a}^\dagger_x)$$

Bose-Hubbard

O(2): Unmuth-Jockey et al. 16

the second term is small and removes degeneracy of the otherwise non-interacting ground state (degenerate pert. theory)
Intermezzo: Entanglement

(later an observable and the basis for the MPS approach)

eample: qubits $A$ and $B$, each in $\{\ket{0}, \ket{1}\}$

states of the combined system:

- $|ψ⟩ = \frac{1}{\sqrt{2}} (|00⟩ \pm |11⟩)$
  
  “if Bob measures and finds 0 (or 1), then Alice finds 0 (or 1) with certainty”

  maximally entangled (very nonclassical)

- $|ψ⟩ = |00⟩$

  “Alice finds 0 irrespective of Bob”: not entangled

- $|ψ⟩ = \frac{1}{2} (|00⟩ + |01⟩ + |10⟩ + |11⟩)$

  “Alice finds 0 (or 1) with probability 1/2 irrespective of Bob”

  not entangled either, since

  $|ψ⟩ = \frac{1}{\sqrt{2}} (|0⟩ + |1⟩)_A × \frac{1}{\sqrt{2}} (|0⟩ + |1⟩)_B$ is actually a product state
how strong are the nonclassical correlations between subsystems? how to measure the deviation from a product state?

- recall: (exp. value $\langle \hat{A} \rangle = \text{tr}(\rho \hat{A})$ for operator $\hat{A} = -\log \rho$)

\[
S = -\text{tr}(\rho \log \rho) \quad \ldots \text{entropy}
\]

\[
\rho = \sum_i p_i |\phi_i\rangle\langle \phi_i| \quad \ldots \text{density matrix, } p_i \in [0, 1], \sum_i p_i = 1
\]

vanishes for a pure state

- for a subsystem $A$ and its complement $B$ define: von Neumann

\[
S_A := -\text{tr}(\rho_A \log \rho_A) \quad \ldots \text{entanglement entropy}
\]

\[
\rho_A := \text{tr}_B |\psi\rangle\langle \psi| \quad \ldots \text{reduced density matrix}
\]

- typical choice: $A$ and $B$ are half the system
\[ S_A := -\text{tr}(\rho_A \log \rho_A) \quad \ldots \text{entanglement entropy} \]

\[ \rho_A := \text{tr}_B |\psi\rangle\langle \psi| \quad \ldots \text{reduced density matrix} \]

properties:

- \( S_A = 0 \) for a product state \(|\psi\rangle = |\phi\rangle|\eta\rangle \) since \( \rho_A = |\phi\rangle\langle \phi| \cdot 1 \)
- calculation:

\[
S_A = -\sum_i \lambda_i \log(\lambda_i)
\]

where \( \lambda_i \) are the eigenvalues of \( \rho_A \), thus \( \lambda_i \in [0, 1] \), \( \sum_i \lambda_i = 1 \)

the nonnegative summand \(-\lambda \log(\lambda)\) vanishes at \( \lambda = 0 \) and \( \lambda = 1 \)

- for the maximally entangled state of 2 qubits: \( S_A = \log_2 2 = 1 \)

= number of entangled qubits
Explicit ground states at strong coupling

- **$Q = 0$:** $|\psi_0\rangle = |0, 0, \ldots, 0\rangle \Rightarrow S_{N/2} = 0$

- **$Q = 1$:** $|\psi_0\rangle = \frac{1}{\sqrt{N}} (|1, 0, \ldots, 0\rangle + \text{shifts}) \Rightarrow S_{N/2} = 1$

The entanglement entropy of the ground state does not scale with the volume, but rather with the surface area.

Here 2 points instead of proportional to $N/2$

- A theorem for local and **gapped** Hamiltonians in 1+1d  
  
  $\text{Hastings 07}$

- **$Q = 2$:**

  
  $|\psi_0\rangle = c_0(N)(|1, 1, 0, \ldots, 0\rangle + \text{shifts}) + c_1(N)(|1, 0, 1, \ldots, 0\rangle + \text{shifts}) + c_2(N)(|1, 0, 0, 1, \ldots, 0\rangle + \text{shifts}) + \ldots$

  
  $S_{N/2} \xrightarrow{N \to \infty} 1.35$

  
  Analytically for small $N$'s: $c_0 < c_1 < c_2 \ldots$
Matrix product states

\( N \) systems with \( d \) levels ("qudits")

- general state: \( |\psi\rangle = \sum_{i_1,..,i_N=0}^{d-1} c_{i_1,..,i_N} |i_1\rangle .. |i_N\rangle \)

\( c \) has \( d^N \) complex entries = effort grows exp. with the volume

\( \Rightarrow \) not necessary when seeking ground states

- Matrix Product States:

\[
|\psi\rangle = \sum_{i_1,..,i_N=0}^{d-1} \text{tr} A_1^{(i_1)} A_2^{(i_2)} .. A_N^{(i_N)} |i_1\rangle .. |i_N\rangle
\]

connect nearest neighbors:

\[
|\ldots\rangle_1 \quad |\ldots\rangle_2 \quad \cdots \quad |\ldots\rangle_N
\]

\( i_1 \quad i_2 \quad \text{index} \quad i_N \)

\( c \quad \text{contractions} \quad A_1 \quad A_2 \quad \cdots \quad A_N \quad \text{matrix} \quad \text{contractions} \)
Matrix Product States:

\[ |\psi\rangle = \sum_{i_1,..,i_N=0}^{d-1} \text{tr} A^{(i_1)}_1 A^{(i_2)}_2 \cdots A^{(i_N)}_N |i_1\rangle \cdots |i_N\rangle \]

\( A \)'s are matrices of dim. \( D \times D \): bond dimension

\( A \)'s have \( d \cdot D^2 \) complex entries altogether = restriction

- extreme case \( D = 1 \): only product states \( \Rightarrow S = 0 \)
- general \( D \): MPS have entanglement entropies bounded by \( \log D \)
- extreme case \( D = O(e^V) \): all states covered
O(3) model through Matrix product states

- coupling $1/g$ determines the lattice spacing (as in QCD)
- $N$ sites = finite volume

MPS:

$$|\psi\rangle = \sum_{j_1, \ldots, j_N=0}^{j_{\text{max}}} \sum_{m_1=-l_1} \sum_{m_N=-l_N} \text{tr} A_1^{(j,m)_1} A_2^{(j,m)_2} \cdots A_N^{(j,m)_N} |(j,m)_1\rangle \cdots |(j,m)_N\rangle$$

$j_{\text{max}} = 1, 2, 3, 4$ (4, 9, 16, 25 states per site) is a truncation to be checked, in addition to the bond dimension $D = O(100)$ of the $A$'s

- we use open boundary conditions which are slightly simpler
- ground and excited state by Rayleigh-Ritz variation principle sweeping through all $A$'s iteratively
Preliminary results: mass gap

- strong coupling regime: perfect
- weak coupling regime = continuum limit:
  - truncations in $j_{\text{max}}$ and finite size seem ok
  - dependence on $D$ to be clarified: critical system
  - effects of open boundary conditions?
Preliminary results: nonzero $\mu$ and charge

- Silver blaze until the mass gap (at that parameter set)
- then particles induced one by one at more critical $\mu_c$’s
  in large volumes these move together to form a quantum phase transition inducing particle density

  $1/g=1.0$

- sharpens with bond dimension $D$
- $1/g$ to be moved closer to continuum scaling

FB et al. 16
Preliminary results: nonzero $\mu$ and charge

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FB et al. 16

- sharpens with bond dimension $D$
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Summary

Matrix Product States

grouped entanglement entropies scaling with log $D$ (bond dimension)
to capture ground states of local gapped Hamiltonians (area law)

- no sign problem in Hamiltonian formulation

in O(3) model: angular momentum + hopping

- strong coupling = effectively qubits
  analytic ground states in charge sectors: indeed $S_{N/2} \to \text{const.}$

- weak coupling = critical system
  check $D$-dependence, otherwise comparable to other approaches

- nonzero $\mu$
  sharp transitions to integer charges

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O(3) model at nonzero density through matrix product states
Outlook

- in progress: central charge from $S_A$ scaling with the size of $A$

- periodic boundary conditions
- nonzero temperature
- higher $O(N)$ or $CP(N)$ models
- higher dimensions
  - Projected Entangled Pair States (PEPS)
- gauge theories

Schwinger model: Banuls et al. 16

<your wish could be here> stay tuned
motivation: sign problem representation-dependent

- weights factorize if action “brought down” by expansion:

\[ e^{-S} \sim \prod_{x,\nu} e^{J n_3(x)n_3(x+\hat{\nu})} = \prod_{x,\nu} \sum_{k_\nu(x)=0}^{\infty} \frac{J_{\nu}(x)}{k_\nu(x)!} (n_3(x)n_3(x + \hat{\nu}))^{k_\nu(x)} \]

\[ \times \sum_{k_\nu^\pm(x)=0}^{\infty} \frac{J_{\nu^\pm}(x)}{k_\nu^\pm(x)!} \left( \ldots (x) \ldots (x + \hat{\nu}) \right)^{k_\nu^\pm(x)} \]

- integrating out all U(1) phases (sign problem!) gives constraints:

\[ \sum_{\nu} \left[ k_{\nu}^+(x) - k_{\nu}^-(x) - (x \Leftrightarrow x + \hat{\nu}) \right] = 0 = \sum_{\nu} \nabla_{\nu} m_\nu(x) \]

= manifest conservation of the U(1) current \( m = k^+ - k^- \)

- chemical potential couples to corresponding charge:

\[ e^{\mu \sum_x m_0(x)} = e^{a_\mu N_t \sum_{\vec{x}} m_0(x)} = e^{\mu/T} Q \]

- all other terms positive \( \Rightarrow \) sign problem solved
Back-up: Results of dual variable simulations with worm algorithm at small $T$:

- **Silver Blaze till dyn. mass $m$**
- then second order quantum phase transition ($T = 0$)
- comparison to Lieb-Liniger and free fermions

- particles induced one by one
- sharp jump at $\mu_{c,2} = E_{\text{min},Q=2}$
  $\Rightarrow$ interactions (phase shifts) 
  a la Lüscher