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

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[in progress]

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The O(3) model in 2d

$$S = \frac{1}{2g}\int d^2x\,(\partial_\nu \vec{n})^2\,, \qquad \vec{n}\in S^2$$

as an important toy model for 4d QCD:

- asymptotically free = negative β-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 $n_1 + in_2 = n_{12}$:

$$S = -\frac{1}{g}\sum_{x,\nu}\Big[n_3(x)n_3(x+\hat{\nu}) + \frac{1}{2}\,n_{12}^*(x)n_{12}(x+\hat{\nu}) + \frac{1}{2}\,n_{12}(x)n_{12}^*(x+\hat{\nu})\Big]$$

- nonzero chem. potential for one global $O(2) = U(1)$:

$$n_3(x)n_3(x+\hat{\nu}) + \frac{1}{2}n_{12}^*(x)n_{12}(x+\hat{\nu})e^{\mu\,\delta_{\nu,0}} + \underbrace{\frac{1}{2}n_{12}(x)n_{12}^*(x+\hat{\nu})e^{-\mu\,\delta_{\nu,0}}}_{\text{not c.c.}}$$

  action not real $\Rightarrow$ sign problem

- exact transformation to dual variables ▸ details

  positive weights $\Rightarrow$ sign problem solved ▸ num. results

  FB, Kloiber, Gattringer, Sulejmanpasic 14-16

▶ Hamiltonian approach

aim: $T = 0$ physics at varying μ by determining the ground states

Hamiltonian approach to the O(3) model

Hamilton operator: Hamer, Kogut, Susskind 78

- kinetic term of a vector $\vec{n}$ on $S^2 \equiv$ orbital angular momentum

  chemical potential (magnetic field) couples to 3rd component

  $\hat{H} \sim \hat{\vec{J}}^2, \mu \hat{J}_z$

- 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 $\hat{\vec{n}}$ in $|j,m\rangle$ Wigner-Eckart

$$\langle j,m| \left\{ \begin{matrix} \hat{n}_{12} \\ \hat{n}_{12}^\dagger \\ \hat{n}_3 \end{matrix} \right\} |j',m'\rangle \sim \underbrace{\langle j,0;1,0|j'0\rangle \cdot \langle j,-m;1,\left\{ \begin{matrix} +1 \\ -1 \\ 0 \end{matrix} \right\} |j',m'\rangle}_{\text{Clebsch-Gordons (real)}}$$

  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 $\hat{\vec{n}}$ and its commuting algebra are violated mildly

Ground state of the O(3) model

in sector Q at strong coupling

- leading Hamiltonian:

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

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

- charge $Q = \sum_x \hat{J}_{z,x} \to \sum_x m_x$ needs $(j,m)_x = (1,1)$ at Q sites
- effectively qubits: occupation numbers "0" or "1" with Hamiltonian

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

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

for newcomers like me

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

example: qubits A and B, each in $\{|0\rangle, |1\rangle\}$

states of the combined system:

- $|\psi\rangle = \frac{1}{\sqrt{2}}\big(|00\rangle \pm |11\rangle\big)$

  "if Bob measures and finds 0 (or 1), then Alice finds 0 (or 1) with certainty"

  maximally entangled (very nonclassical)

- $|\psi\rangle = |00\rangle$

  "Alice finds 0 irrespective of Bob": not entangled

- $|\psi\rangle = \frac{1}{2}\big(|00\rangle + |01\rangle + |10\rangle + |11\rangle\big)$

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

  not entangled either, since

  $|\psi\rangle = \frac{1}{\sqrt{2}}\big(|0\rangle + |1\rangle\big)_A \times \frac{1}{\sqrt{2}}\big(|0\rangle + |1\rangle\big)_B$ 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 $\langle \hat{A} \rangle = \mathrm{tr}(\rho \hat{A})$ for operator $\hat{A} = -\log \rho$)

$$S = -\mathrm{tr}(\rho \log \rho) \qquad \ldots \text{entropy}$$

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

vanishes for a pure state

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

$$S_A := -\mathrm{tr}(\rho_A \log \rho_A) \qquad \ldots \text{entanglement entropy}$$

$$\rho_A := \mathrm{tr}_B \, |\psi\rangle\langle\psi| \qquad \ldots \text{reduced density matrix}$$

- typical choice: A and B are half the system

$$S_A := -\mathrm{tr}(\rho_A \log \rho_A) \qquad \ldots \text{entanglement entropy}$$
$$\rho_A := \mathrm{tr}_B |\psi\rangle\langle\psi| \qquad \ldots \text{reduced density matrix}$$

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 λ_i are the eigenvalues of ρ_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

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

  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   Hastings 07
- $Q = 2$:

$$
\begin{aligned}
|\psi_0\rangle = {} & c_0(N)\big(|1,1,0,\ldots,0\rangle + \text{shifts}\big) \qquad S_{N/2} \xrightarrow{N\to\infty} 1.35 \\
& + c_1(N)\big(|1,0,1,\ldots,0\rangle + \text{shifts}\big) \\
& + c_2(N)\big(|1,0,0,1,\ldots,0\rangle + \text{shifts}\big) + \ldots
\end{aligned}
$$

  analytically for small N's: $c_0 < c_1 < c_2 \ldots$

Matrix product states

N systems with d levels ("qudits")

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

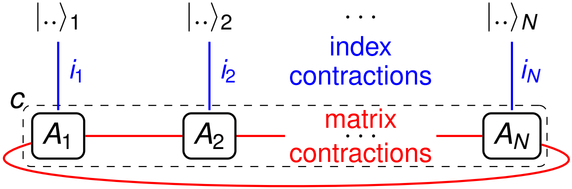
  c has d^N complex entries = effort grows exp. with the volume

$\Rightarrow$ not necessary when seeking ground states

- Matrix Product States:

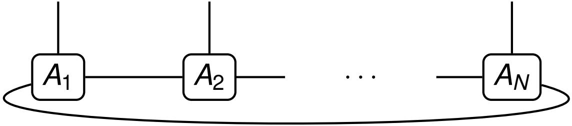
$$|\psi\rangle = \sum_{i_1,..,i_N=0}^{d-1} \operatorname{tr} A_1^{(i_1)} A_2^{(i_2)} .. A_N^{(i_N)} \, |i_1\rangle..|i_N\rangle$$

  connect nearest neighbors:



- Matrix Product States:

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



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 $D = \mathcal{O}(e^V)$: all states covered

O(3) model through Matrix product states

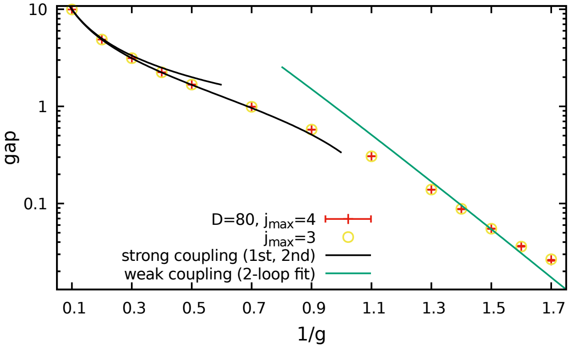
- coupling $1/g$ determines the lattice spacing (as in QCD)
- N sites = finite volume
- MPS:

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

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

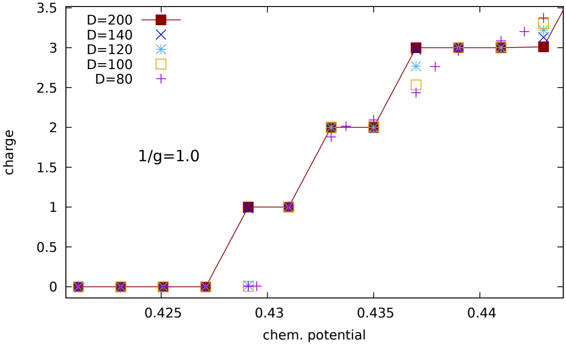
- we use open boundary conditions which are slightly simpler
- ground and excited state by Rayleigh-Ritz variation principle sweeping through all A's iteratively

Preliminary results: mass gap



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

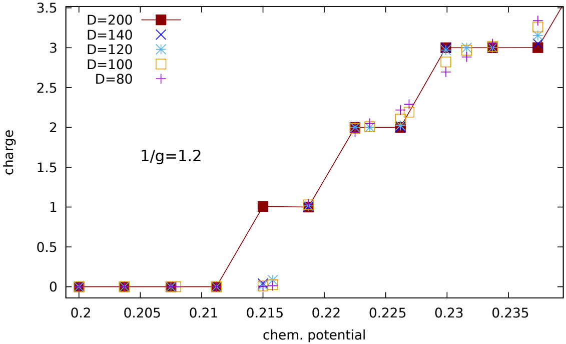
Preliminary results: nonzero μ and charge



- Silver blaze until the mass gap (at that parameter set)
- then particles induced one by one at more critical μ_c's

  in large volumes these move together to form a quantum phase transition inducing particle *density* FB et al. 16
- sharpens with bond dimension D
- $1/g$ to be moved closer to continuum scaling

Preliminary results: nonzero μ and charge



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Summary

Matrix Product States talk by N. Schuch

- small 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 $S_{N/2} \to$ const.
- weak coupling = critical system
  check D-dependence, otherwise comparable to other approaches
- nonzero μ
  sharp transitions to integer charges

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

Back up: dual variables in a nutshell

$\approx$ Kramers, Wannier 41

motivation: sign problem representation-dependent

- weights factorize if action "brought down" by expansion:

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

$$\times \sum_{k_\nu^{\pm}(x)=0}^{\infty} \frac{J^{k_\nu^{\pm}(x)}}{k_\nu^{\pm}(x)!} \left(\ldots(x) \ldots (x+\hat{\nu}) \right)\Big)^{k_\nu^{\pm}(x)}$$

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

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

= 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

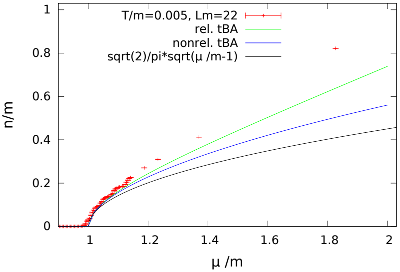
Prokof'ev, Svistunov 01

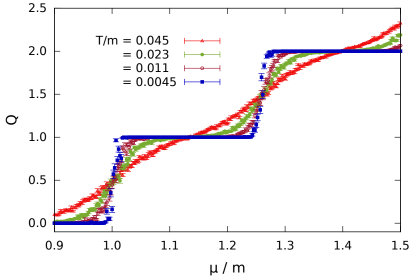
at small T:

lattices $N_t \times N_s$ up to 6400×160

large volumes

smallish volumes $(Lm = 4.4)$





- 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 $\mu_{c,2} = E_{\min,Q=2}$

$\Rightarrow$ interactions (phase shifts)

a la Lüscher