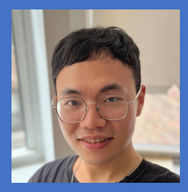
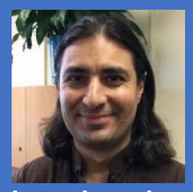

Bond-dependent slave-particle cluster theory based on density matrix expansion

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Prior slave-particle (SP) methods [1-4]

Hubbard model $\hat{H} = -\sum_{ij\sigma} t_{ij\sigma}\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + \sum_{i\sigma}\epsilon_{i\sigma}\hat{n}_{i\sigma} + \sum_i \hat{H}^{int}_i$

Physical indices: Site: i, j; Spin: σ, σ'; Greek-letter combine site and spins: $\alpha \equiv i\sigma$

Electron $\hat{c}$ → Hilbert space $\mathcal{H} \to \mathcal{H}_f \otimes \mathcal{H}_s$ (Decouple spin and charge) → Spin $\hat{f}$: Non-interacting spinon; Charge $\hat{O}$: Interacting auxiliary SP (need further approximation)

- **Local SP operators** defined from $\hat{c}_\alpha \to \hat{f}_\alpha \hat{O}_\alpha$.

Where SP operator $\hat{O}_\alpha \equiv \begin{pmatrix} 0 & 1 \\ C_\alpha & 0 \end{pmatrix}$ on SP number basis $|N^s_\alpha = 0\rangle, |N^s_\alpha = 1\rangle$ ensures anticommutation relation hold for electrons and spinons for arbitrary gauge number C_α (calibrated by non-interacting limit in practice).

- **Standard single-site approximation** $\langle \hat{O}^{\dagger}_\alpha \hat{O}_\beta \rangle = \langle \hat{O}^{\dagger}_\alpha \rangle \langle \hat{O}_\beta \rangle$ when α, β are on different sites

Better SP operators

With local SP operators, hopping operator $\hat{O}^{\dagger}_\alpha \hat{O}_\beta + h.c.$ unphysically changes particle number by ± 2.

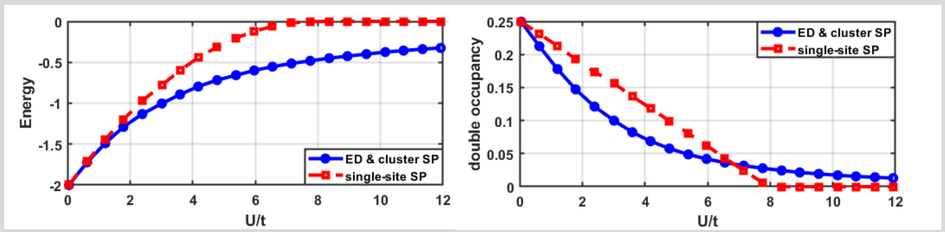
We introduce novel **nonlocal SP operators defined on bonds**, where additional bond index $\langle\alpha\beta\rangle$ is added into the SP operators.

$$\hat{c}^{\dagger}_\alpha \hat{c}_\beta \to \hat{f}^{\dagger}_\alpha \hat{f}_\beta \hat{O}^{\dagger}_{\alpha\langle\alpha\beta\rangle}\hat{O}_{\beta\langle\alpha\beta\rangle}$$

With this framework, all **unphysical hoppings are now forbidden** by the simple constraints $C_{\alpha\langle\alpha\beta\rangle} + C_{\beta\langle\alpha\beta\rangle} = 0$ on each bond$\langle\alpha\beta\rangle$.

Better approximation to SP problem

Single-site method predicts a wrong Mott transition in 1D half-filled Hubbard model.

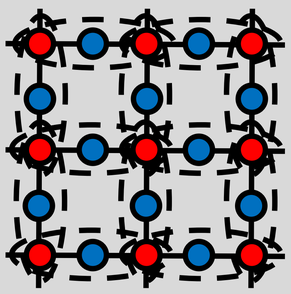


Shown above is the Hubbard dimer calculated with single-site SP method (energy in units of hopping t) as a function of interaction strength U/t. Single-site method predicts a wrong Mott transition at $U = 8t$, which is absent in exact diagonalization (ED).

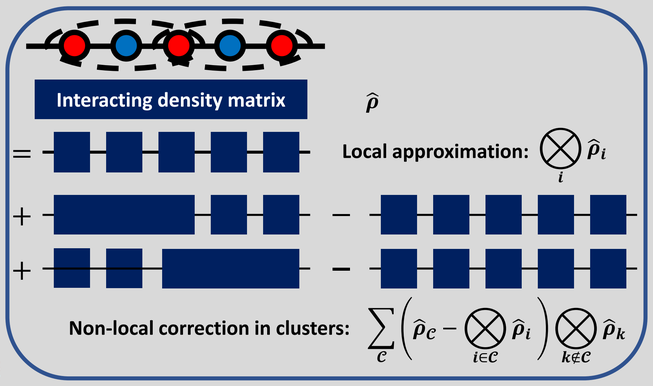
We introduce a **new cluster SP method** based on the **expansion of the SP lattice density matrix** into a set of overlapping clusters in real space.

$$\hat{\rho} = \bigotimes_i \hat{\rho}_i + \sum_C \left(\hat{\rho}_C - \bigotimes_{i\in C} \hat{\rho}_i \right) \bigotimes_{k\notin C} \hat{\rho}_k$$

Where i, k are site indices and C is the cluster index. A good choice of cluster is a dpd cluster marked by dashed ellipse below in a dp model, where d-sites are in red and p-sites are in blue. Our method reproduces the exact ED results for a Hubbard dimer cluster.



- No averaged bath
- No left out chemical bonds



Minimization problem with constraints

Minimize total energy:

$$E = -\sum_{\alpha\beta} t_{\alpha\beta} \langle \hat{f}^{\dagger}_\alpha \hat{f}_\beta \rangle_{\rho_f} \left\langle \hat{O}^{\dagger}_{\alpha\langle\alpha\beta\rangle}\hat{O}_{\beta\langle\alpha\beta\rangle} \right\rangle_{\rho_s} + \sum_\alpha \epsilon_\alpha \langle \hat{n}_\alpha \rangle_{\rho_f} + \sum_i U_i \langle \hat{N}_{i\uparrow}\hat{N}_{i\downarrow} \rangle_{\rho_s}$$

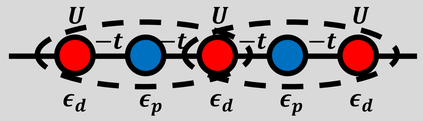
With constraints:

- Number matching between spinon and SP $\langle \hat{n}_\alpha \rangle_{\rho_f} = \langle \hat{N}_\alpha \rangle_{\rho_s}$

Gauge constraints:

- Spinons recovers electrons in non-interacting limit $\left\langle \hat{O}^{\dagger}_{\alpha\langle\alpha\beta\rangle}\hat{O}_{\beta\langle\alpha\beta\rangle} \right\rangle_{\rho_s} = 1$
- Unphysical hoppings are forbidden: $C_{\alpha\langle\alpha\beta\rangle} + C_{\beta\langle\alpha\beta\rangle} = 0$

Tests on one-dimensional dp model



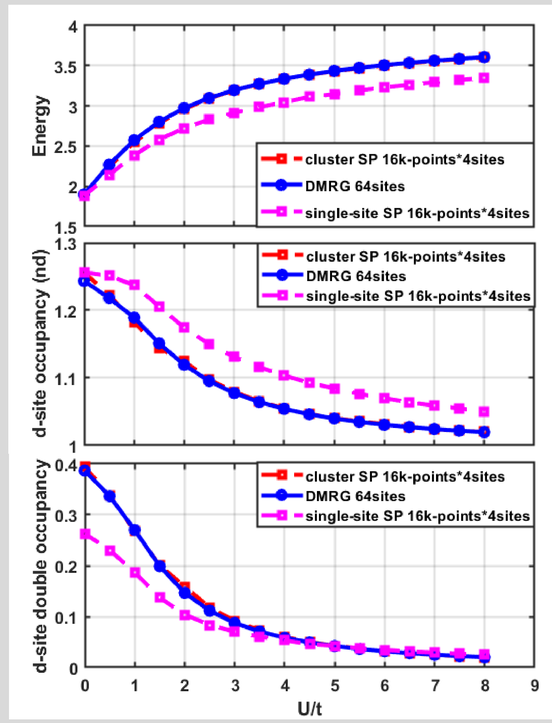
Onsite energy $\epsilon_d - \epsilon_p = 2t$

Number of electrons $N_e = N_{d-sites} + 2N_{p-sites}$

Ground state energy per four-site unit cell in unit of t (2 d- and 2 p-sites)

d-site occupancy $\langle \hat{n}_d \rangle = \langle \hat{n}_{d\uparrow} + \hat{n}_{d\downarrow} \rangle$

d-site double occupancy $D = \langle \hat{N}_{d\uparrow}\hat{N}_{d\downarrow} \rangle_{\rho_s}$



Calculations performed on a 64-site dp system with PBC

Cluster SP theory in one-dimensional dp model:

- Straightforward implement of translational symmetry in non-interacting spinon by k-sampling
- Remarkable accuracy comparing with density matrix renormalization group (DMRG) benchmark (using ITensors package [5])
- Great improvement to previous SP methods [1-4] based on single-site approximation (using BoSS software [6])

Reference

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[5] M. Fishman et al., arXiv:2007.14822
Website: https://itensor.github.io/ITensors.jl/stable/index.html
[6] A. B. Georgescu et al., Computer Physics Communications 265, 107991 (2021)
Website: https://bitbucket.org/yalebosscode/boss/wiki/Home

Self-consistent effective Hamiltonians

Non-interacting spinon

$$H_f = -\sum_{\alpha\beta} t_{\alpha\beta} \left\langle \hat{O}^{\dagger}_{\alpha\langle\alpha\beta\rangle}\hat{O}_{\beta\langle\alpha\beta\rangle} \right\rangle_{\rho_s} \hat{f}^{\dagger}_\alpha \hat{f}_\beta + \sum_\alpha (\epsilon_\alpha + h_\alpha{}')\hat{n}_\alpha$$

Interacting auxiliary SP in clusters

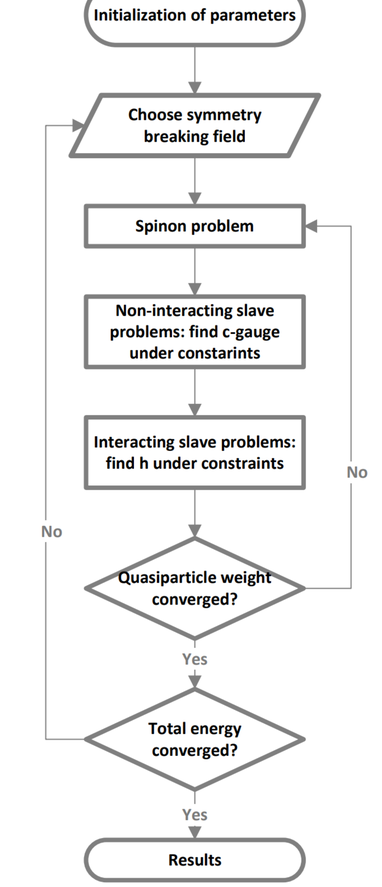
$$H_{\mathcal{C}} = -\sum_{\substack{\alpha\beta \\ \langle\alpha\beta\rangle\in\mathcal{C}}} t_{\alpha\beta} \langle \hat{f}^{\dagger}_\alpha \hat{f}_\beta \rangle_{\rho_f} \hat{O}^{\dagger}_{\alpha\langle\alpha\beta\rangle}\hat{O}_{\beta\langle\alpha\beta\rangle}$$
$$- \sum_{\substack{\alpha\beta \\ \alpha\in\mathcal{C},\beta\notin\mathcal{C}}} \frac{t_{\alpha\beta}}{M_\alpha} \langle f^{\dagger}_\alpha f_\beta \rangle_{\rho_f} \left[\left\langle O^{\dagger}_{\beta\langle\alpha\beta\rangle} \right\rangle_{\rho_\alpha} O_{\alpha\langle\alpha\beta\rangle} + h.c. \right]$$
$$+ \sum_{i|i\in\mathcal{C}} \frac{1}{M_i} \left(U_i N_{i\uparrow} N_{i\downarrow} + \sum_\sigma h_{i\sigma\mathcal{C}} N_{i\sigma} \right)$$

$h_{i\sigma\mathcal{C}}$: Lagrange multipliers
$h_\alpha{}'$: symmetry breaking field and Lagrange multipliers
M_i (or M_α): the number of clusters containing site i

Self-consistent hopping renormalization factors:

$$\left\langle \hat{O}^{\dagger}_{\alpha\langle\alpha\beta\rangle}\hat{O}_{\beta\langle\alpha\beta\rangle} \right\rangle_{\rho_s}, \left\langle O^{\dagger}_{\beta\langle\alpha\beta\rangle} \right\rangle_{\rho_\alpha}, \langle \hat{f}^{\dagger}_\alpha \hat{f}_\beta \rangle_{\rho_f}$$

Workflow



Future directions

- Higher dimensional systems
- Multiple orbitals on each site
- Excited states and time evolution
- More observables: spectrums, correlations etc.

Related 2022 March meeting talk A48.00008: Bond-dependent slave-particle cluster theory
https://apsmarch22.onlineeventpro.freeman.com/sessions/23877948/subsession/31536084/A48

Related talk by Sohrab Ismail-Beigi: Session 8