From variational ansatz to 'exact' results: a numerical exploration of models of strongly correlated systems

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GORDON AND BETTY MOORE FOUNDATION

Outline

Non-fermi liquid <—> Ground state for ring-exchange Hamiltonian

Suggestions of Pseudogap

VMC Wavefunctions
- AFM + Backflow
- Breaking symmetry in Slater-Jastrow
- Finite PEPS

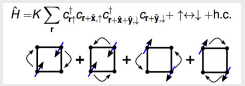
New Methods
- Shift and Inverse MPS (SIMPS) <—> Access to excited states
- Stochastic Evolution MPS (SEMPS)
- Tensor Networks + QMC

Ring Exchange Hamiltonian

with Katie Hyatt and Matthew Fisher

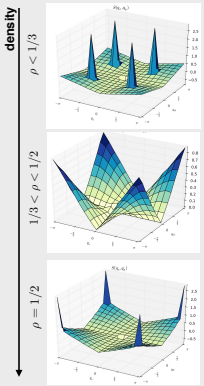
tjk model with t=J=0

$\hat{H} = K \sum_r c^\dagger_{r\uparrow} c_{r+\hat{x}+\hat{y},\uparrow} c^\dagger_{r+\hat{x},\downarrow} c_{r+\hat{y},\downarrow} + \uparrow\leftrightarrow\downarrow + \text{h.c.}$



sign-problem free
- can access 2D system
- technically difficult; dimer-like
- use Diffusion Monte Carlo + forward walking

conserved quantum numbers
- electrons per row
- Sz parity per sublattice



phase separation: 'stripes'

Exciton Bose-liquid (EBL) in charge sector
Bose surface of gapless excitations
Smoking gun of EBL

charge density wave

References

Backflow: Feynman; Sorella, et. al; Holzmann, et. al;

SIMPS: http://arxiv.org/pdf/1509.01244.pdf

EBL: Paramekanti, L. Balents, M. P. A. Fisher, Phys.Rev. B66, 054526 (2002).

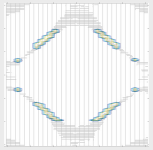
PEPS: Bauer, et. al; Corboz, et. al

Pseudogap?

with Xiongjie Yu

Preliminary suggestion of pseudogap? superconductivity?

dn(k)/dk
possibly metastable
filling ~ 0.84; 4x32; DMRG



VMC on Hubbard

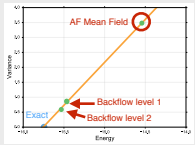
with Han-Yi and Xiongjie Yu

Why VMC? Because VMC gives insight into the nature of your wave-function.

Q: Can simple variational wave-functions teach us something about the important physics.

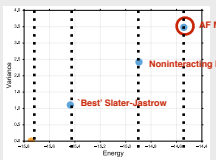
For concreteness, let's consider small systems at U=4 and filling ~ 0.875.

AFM + (better) backflow extrapolate to the right energy (on small systems)

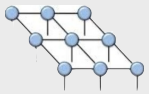


Backflow: $Det[\phi_i(r_j)]e^J$
$r_i \to q_i(r_i; R)$ or
$\phi_i(r_j) \to \tilde{\phi}_i(r_j)$

Allowing arbitrary breaking of symmetries helps.



Low bond-dimension PEPS helps a bit…



PEPS-alone (D=2): -10.6

PEPS-Slater-Jastrow (D=2): -15.44

Optimization via Monte Carlo:
- Imaginary time evolution
- Stochastic Reconfiguration
- Exact linear sweeping

3-band (and others) with VMC, SEMPS, PEPS, AFQMC, DMET … coming soon

SEMPS

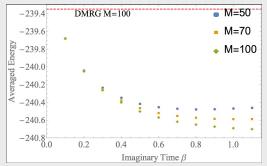
with Xiongjie Yu

SEMPS (Stochastically evaluating matrix product states)

Quantum Monte Carlo: *Stochastic Imaginary Time Evolution* [Sign Problem!]

Matrix Product States: *Deterministic Imaginary Time Evolution* [Finite Bond Dim.]

Combination: (1) Start with a good wave-function.
(2) Sample configurations from it
(3) Imaginary time evolve MPS from these deterministically.
(4) When you run out of bond-dimension, resample from these (this can be done exactly)

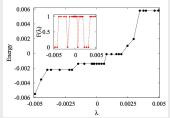


SIMPS

with Xiongjie Yu and David Pekker

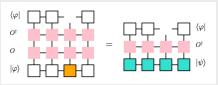
SIMPS (Shift and Invert MPS) allows the finding of eigenstates in the matrix-product state formalism - works with $(H\text{-}E)^{-1}$

This gives us a new way to target excited states at energy E.



$$\frac{\partial}{\partial \varphi^*_{i,\sigma}} ||O|\varphi\rangle - |\psi\rangle||^2 = 0,$$

$$\frac{\partial}{\partial \varphi^*_{i,\sigma}} \langle\varphi|O^\dagger O|\varphi\rangle = \frac{\partial}{\partial \varphi^*_{i,\sigma}} \langle\varphi|O^\dagger|\psi\rangle.$$

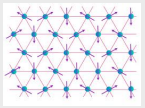


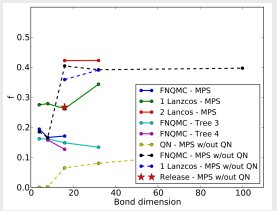
(We also have an alternative approach to this which is a variant to DMRG - ESDMRG)

QMC + Tensor Networks

with Hitesh Changlani

$H = \sum_{\langle i,j \rangle} S_i \cdot S_j$

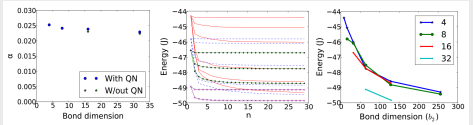


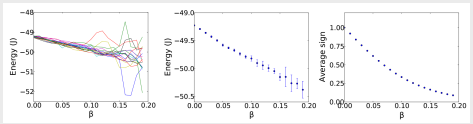


Exact (Stochastic) Projection $|\Psi_0\rangle = \exp[-\beta H]|\Psi_T\rangle$

- Sample R with probability $|\Psi_T(R)|^2$
- Apply $G(R \to R') = (I - \tau H(R,R')) \frac{\Psi(R')}{\Psi(R)}$
- Compute Observables

Cost: $O(D^\alpha)$ per Monte Carlo step





Lanczos++

Basis: $\{|\Psi\rangle, H|\Psi\rangle, H^2|\Psi\rangle, H^3|\Psi\rangle, H^4|\Psi\rangle, ...\}$

Solve: $H|\Psi\rangle = ES|\Psi\rangle$ in this basis

Ways to compute basis

- MPS/MPO Formalism (exact)
- Quantum Monte Carlo (exact)
- Hybrid QMC/MPO (exact)
- Apply $H|\Psi\rangle$ via MPO, truncate to b2 and iterate (approximate)