Wave-functions for improved simulations of strongly correlated systems

Bryan Clark
University of Illinois at Urbana Champaign

A new wave-function

Work with Hassan Shapourian

Computational tools are critical to understanding materials.

Many of those tools depend on a wave-function as input.

For Bosonic systems we find a new type of wave-function which improves upon the current state of the art.

Jastrow wave-function

Typical Approach:

$$\Psi = \prod_{ij} \exp[-U(r_i - r_j)]$$

expand in short-range pair product terms

go to higher order (three-body) terms for further accuracy

* not possible to empty condensate fraction in a Mott Insulator

Parton wave-function

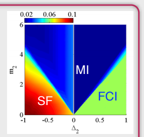
$$\Psi(\{\mathbf{r}_i\}) = \det_1(\{\mathbf{r}_i\}) \times \det_2(\{\mathbf{r}_i\})$$

ground state of non-interacting topological phase

$$H = \sum_{\langle ij \rangle} t_{ij} c_i^\dagger c_j + i \sum_{\langle\langle ik \rangle\rangle} \Delta_{ik} c_i^\dagger c_k + \sum_i m_i c_i^\dagger c_i$$

Can tune (Δ, m)

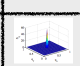
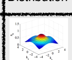
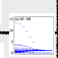
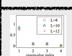
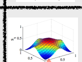
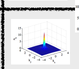
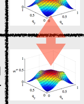
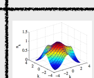
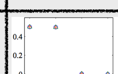
Motivated by analytical theory



f_2 parameters	C_2	bosonic phase
$\Delta_2 > 0, \lvert m_2 \rvert < 4\lvert\Delta_2\rvert$	$+1$	FCI $\nu = 1/2$
$\Delta_2 < 0, \lvert m_2 \rvert < 4\lvert\Delta_2\rvert$	-1	SF
$\lvert m_2 \rvert > 4\lvert\Delta_2\rvert$	0	MI

We've developed a new class of two-parameter wave-functions which accurately describes both landau symmetry breaking phases and topological phases. This puts two very different classes of phases in one framework

How do we know? Use variational Monte Carlo to compute many properties.

	Structure Factor	Momentum Distribution	Topological
Mott Insulator		 	
Superfluid			gapless
Fractional Chern Insulator			

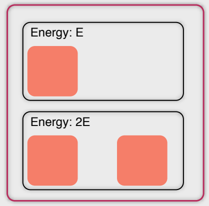
Size consistency

The energy of two identical systems is twice the energy of one system.

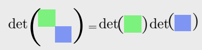
Non-interacting systems, such as Hartree-Fock are size-consistent.

Hard to write down interacting wave-functions which are size-consistent.

The parton wave-functions we write down are size-consistent.



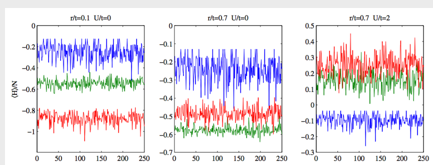
Why?



Predicting a new phase

$$H = -t \sum_{\langle i,j \rangle} (b_i^\dagger b_j + b_j^\dagger b_i) + r \sum_{\langle\langle i,j \rangle\rangle} (b_i^\dagger b_j + b_j^\dagger b_i) + \frac{U}{2} \sum_{\langle i,j \rangle} n_i n_j$$

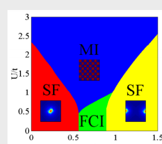
Use variational Monte Carlo to determine energetics.



Superfluid

Fractional Chern Insulator

Mott Insulators



Critical exponents

Transition	Critical point	ν	η
SF-MI (t/U)	0.45 ± 0.04	0.51 ± 0.06	0.64 ± 0.05
SF-FCI (r/t)	0.59 ± 0.02	0.14 ± 0.02	0.58 ± 0.08

Perfect Insulators

Work with David Pekker

Most materials which are insulators, nonetheless have conductivity at finite temperature. Systems that are in the many-body localized (MBL) phases are different - they have exactly zero conductivity even at infinite temperature. These "materials" allow quantum mechanical phenomena to exist at high temperatures and may be useful for a variety of technological applications. They are the interacting analogue of Anderson Insulators. Here we try to numerically simulate and understand the structure of these perfect insulating materials.

Phenomenology

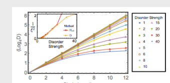
- No conductivity
- No thermalization - statistical mechanics breaks down
- Emergent conserved equations of motion
- No level repulsion of eigenstates
- Eigenstates obey area law

The whole spectrum

$$UHU^\dagger = H_D$$

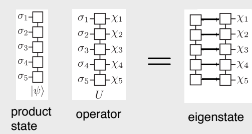
U diagonalizes the spectrum.

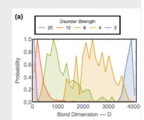
We find a compact representation of U.



Notice U takes a product state and returns an eigenstate.

The MPO Language





The operator is representable by 2n pairs of matrices:
{A1,A2,...,An} and {B1, B2,...,Bn}

Each eigenstates is represented by n of those matrices.
eigenstate 1: {A1,B2,A3,A4,B5,....}
eigenstate 2: {B1,A2,B3,B4,B5,....}

Key question: Are the matrices compact in the MBL?

Important technical point: need to choose a way to match product states to eigenstates locally.

When this is done, matrices are compact!

References

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D. M. Basko, I. L. Aleiner, and B. L. Altshuler, Annals of Physics 321, 1126 (2006)

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We acknowledge support from grant DOE, SciDAC FG02-12ER46875