New Development of Numerical Simulations in Low-Dimensional Quantum Systems:
From Density Matrix Renormalization Group to Tensor Network Formulations

October 27-29, 2010 Yukawa Institute for Theoretical Physics, Kyoto University

Quantum Phase Transitions of Two-Species Bosons

Pochung Chen 陳柏中

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Acknowledgement

- Collaborators:
  - Prof. Min-Fong Yang (Tunghai Univ)
- References:
  - Pochung Chen and Min-Fong Yang, arXiv:1009.2841

Motivation

- Ultra-cold atoms in optical lattices provide a fascinating playground for studying strongly correlated systems
- Single-species boson systems:
  - Superfluid to Mott insulator transition (Observed)
- Two-species boson systems:
  - Exhibit even rich behavior
  - Super CounterFluid (SCF)
  - Pair SuperFluid (PSF)

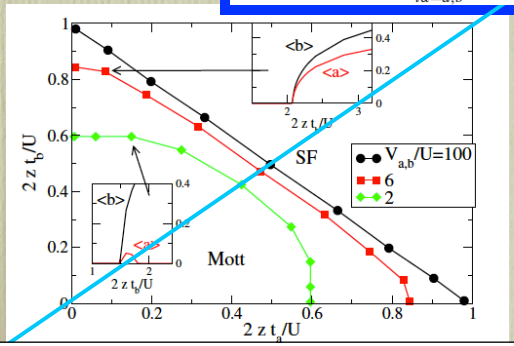
Early Mean Field Study

Phase diagram of two-component bosons on an optical lattice

New Journal of Physics **5** (2003) 113.1–113.19

Ehud Altman, Walter Hofstetter, Eugene Demler and Mikhail D Lukin

$$H = -\sum_{\langle ij\rangle} t_a (a_i^\dagger a_j + \text{h.c.}) - t_b \sum_{\langle ij\rangle} (b_i^\dagger b_j + \text{h.c.}) + U \sum_i (n_{ai} - \tfrac{1}{2})(n_{bi} - \tfrac{1}{2}) + \tfrac{1}{2} \sum_{i\alpha=a,b} V_\alpha n_{\alpha i}(n_{\alpha i} - 1) - \sum_{i\alpha} \mu_\alpha n_{\alpha i}.$$



No PSF/SCF Phase Found !

Mean Field and Monte Carlo Study

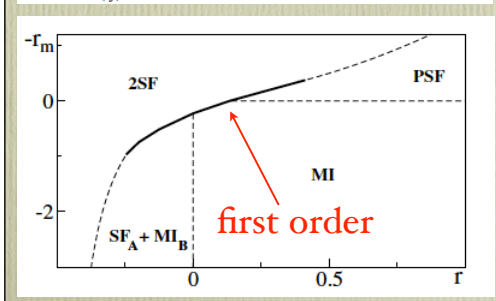
VOLUME 92, NUMBER 5 PHYSICAL REVIEW LETTERS week ending 6 FEBRUARY 2004

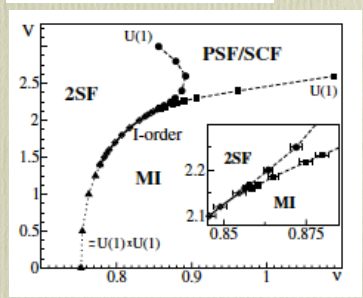
Commensurate Two-Component Bosons in an Optical Lattice: Ground State Phase Diagram

Anatoly Kuklov,[1] Nikolay Prokof'ev,[2,3] and Boris Svistunov[2,3]

$$H = -\sum_{\langle ij\rangle\,\sigma} (t_\sigma a^\dagger_{i\sigma} a_{j\sigma} + \text{H.c.}) + \frac{1}{2}\sum_{i\,\sigma\sigma'} U_{\sigma\sigma'} n_{i\sigma} n_{i\sigma'}.$$

$$S = \sum_{\sigma,\sigma'}\sum_{i} \tilde{U}_{\sigma\sigma'}\, \vec{J}_i^{(\sigma)} \cdot \vec{J}_i^{(\sigma')}.$$





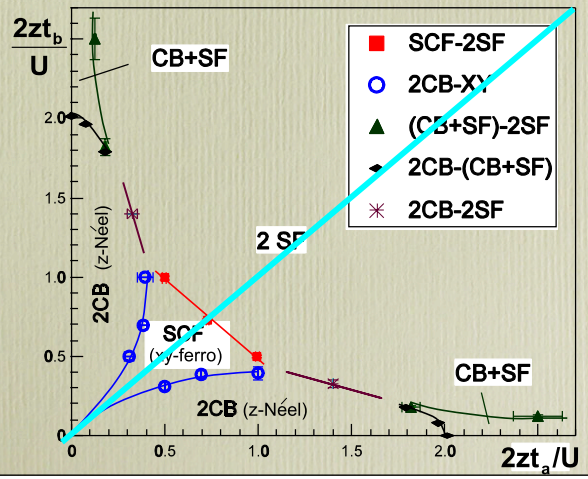
Mean Field

MC (J-current model)

QMC Study (Half-filling)

S. G Söyler, B. Capogrosso-Sansone, N. V. Prokof'ev, B V Svistunov, NJP 11 (2009) 073036

$$H = -\sum_{\langle ij \rangle} \left(t_a a_i^\dagger a_j + t_b b_i^\dagger b_j \right) + U \sum_i n_i^{(a)} n_i^{(b)},$$



Symmetric Hardcore Bosons

$$H = -t\sum_{\langle ij\rangle}\left(a_i^\dagger a_j + b_i^\dagger b_j + h.c.\right) - \mu\sum_{i,\sigma} n_i^\sigma + U_{ab}\sum_i n_i^a n_i^b$$

- Particle-Hole symmetric
- Isotropic hopping
- Possible phases (symmetric around $\mu=-1/2$)
  - MI (Mott Insulating)
  - 2SF (Two SuerFluid)
  - PSF (Paired SuperFluid, $U_{ab}<0$)
  - SCF (Super CounterFluid, $U_{ab}>0$)

Order Parameters

	$\langle a \rangle = \langle b \rangle$	$\langle ab \rangle$	$\langle ab^\dagger \rangle$
MI	0	0	0
2SF	$\neq 0$	$\neq 0$	$\neq 0$
PSF	0	$\neq 0$	0 or $\langle (W_a - W_b)^2 \rangle = 0$
SCF	0	0 or $\langle (W_a + W_b)^2 \rangle = 0$	$\neq 0$

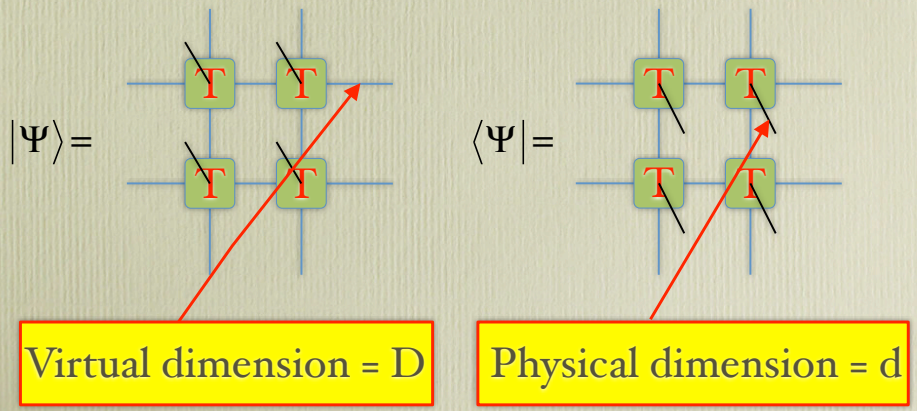
- PSF: $a \to e^{i\theta} a$, $b \to e^{i\theta} b$ broken; $a \to e^{i\theta} a$, $b \to e^{-i\theta} b$ not broken
- SCF: $a \to e^{i\theta} a$, $b \to e^{i\theta} b$ not broken; $a \to e^{i\theta} a$, $b \to e^{-i\theta} b$ broken

The Method

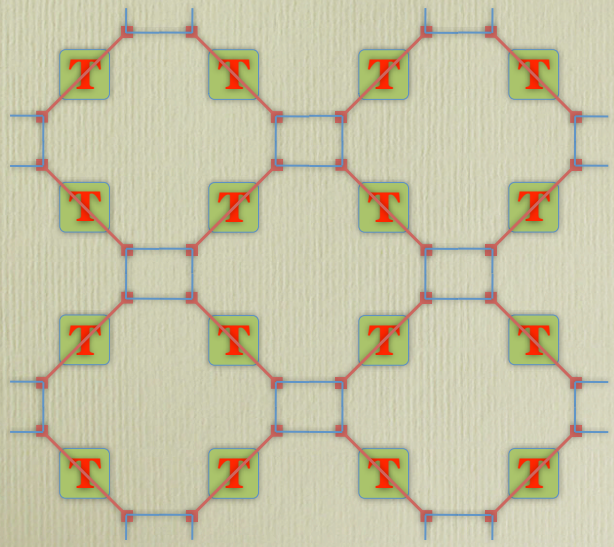
- Wave-function: Tensor Product State (**TPS**)
- Optimization
  - Imaginary time evolution (**Projection**)
    - H. C. Jiang, Z. Y. Weng, and T. Xiang, Phys. Rev. Lett. 101,090603 ,(2008)
- Expectation value
  - Tensor Renormalization Group (**TRG**)
    - M. Levin and C. P. Nave, Phys. Rev. Lett. 99, 120601 (2007)
    - Z.C. Gu, M. Levin, and X. G. Wen, Phys. Rev. B 78, 205116,(2008)

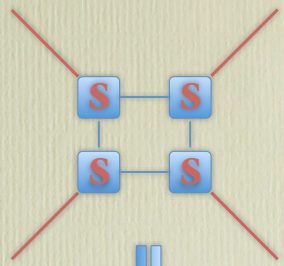
2D Tensor Product State (TPS)

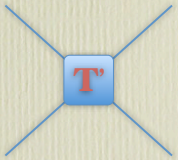
$$|\Psi\rangle = \sum_{S_i S_j \cdots} \mathrm{Tr}\left[T^{S_i}_{u_i l_i d_i r_i} T^{S_j}_{u_j l_j d_j r_j} \cdots \right] |S_i S_j \cdots\rangle$$



Coarse-Grained Tensor Network

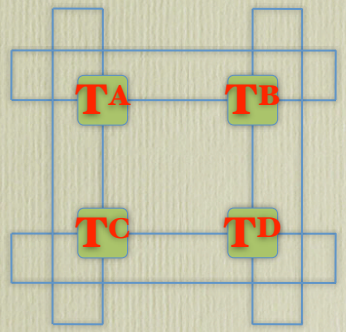






Final 2x2 Plaque

After N iteration of RG, 2x2 plaque effective represent $2^N x 2^N$ lattice
Tensor contract can be done exactly for the 2x2 plaque



Expectation value of TPS can be approximately but efficiently calculated via TERG

Imaginary Time Evolution

- Use imaginary time to reach the ground state
- Assume initial state has some overlap with GS

$$|\psi(0)\rangle = A_0|G\rangle + A_1|E_1\rangle + A_2|E_2\rangle + \cdots$$

- Imaginary time evolution single out the GS

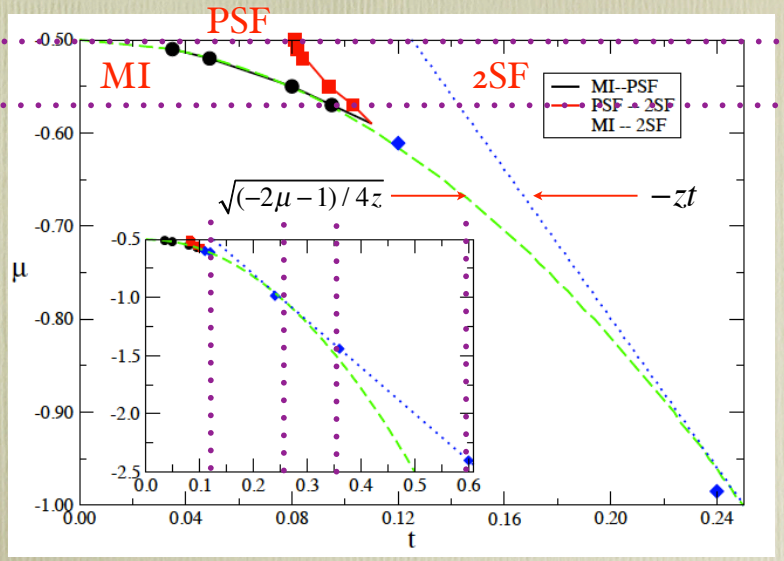
$$e^{-\tau t}|\psi(0)\rangle = A_0|G\rangle + A_1 e^{-\tau E_1}|E_1\rangle + A_2 e^{-\tau E_2}|E_2\rangle + \cdots$$

- Obtain ground state by

$$|G\rangle = \lim_{N\to\infty} \frac{\left(e^{-\delta\tau}\right)^N |\psi(0)\rangle}{\left|\left(e^{-\delta\tau}\right)^N |\psi(0)\rangle\right|}$$

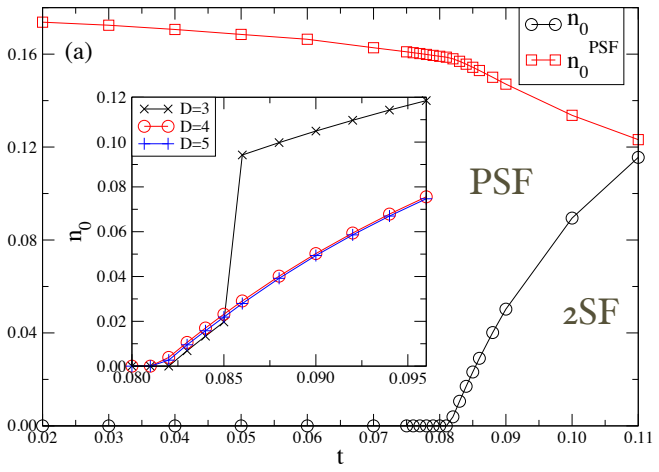
Results

Phase Diagram

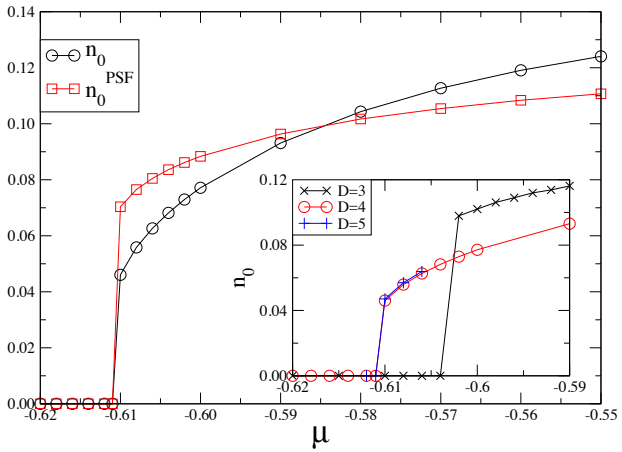


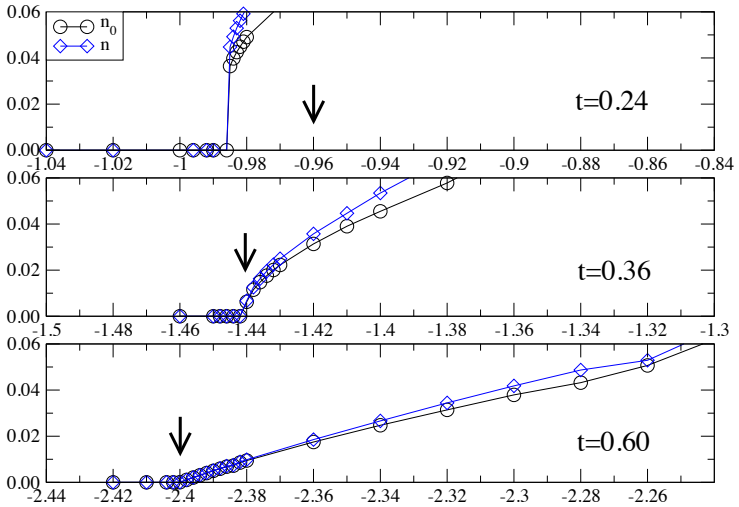
M. Iskin, PRA 82, 033630 (2010)

$\mu = -0.5$

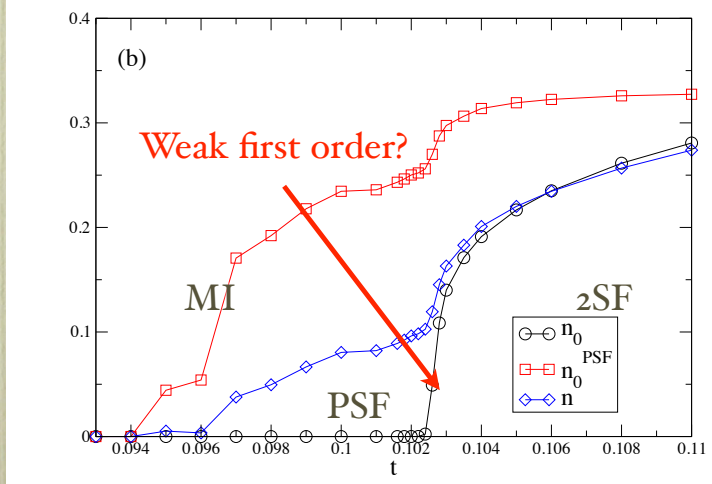


t = 0.12


0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
-0.62
-0.61
-0.60
-0.59
-0.58
-0.57
-0.56
-0.55
μ
n0
n0 PSF
D=3
D=4
D=5
n0
0.12
0.08
0.04
0.00
-0.62
-0.61
-0.6
-0.59


n0
n
t=0.24
t=0.36
t=0.60
0.06
0.04
0.02
0.00
-1.04
-1.02
-1
-0.98
-0.96
-0.94
-0.92
-0.9
-0.88
-0.86
-0.84
-1.5
-1.48
-1.46
-1.44
-1.42
-1.4
-1.38
-1.36
-1.34
-1.32
-1.3
-2.44
-2.42
-2.4
-2.38
-2.36
-2.34
-2.32
-2.3
-2.28
-2.26

$\mu = -0.57$


(b)
Weak first order?
MI
PSF
2SF
n_0
n_0^{PSF}
n
0.4
0.3
0.2
0.1
0
0.094
0.096
0.098
0.1
0.102
0.104
0.106
0.108
0.11
t

Mean Field and Monte Carlo Study

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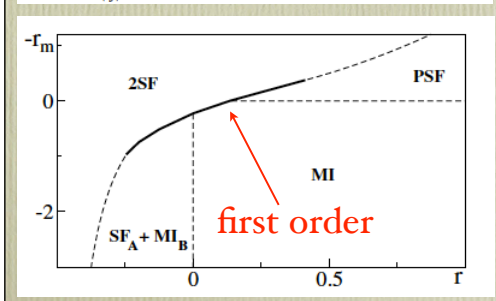
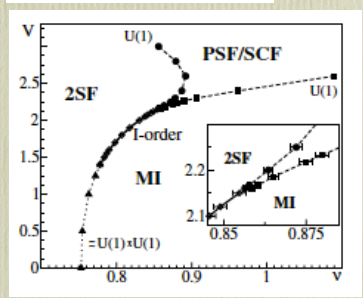




Mean Field

MC (J-current model)

Summary and Outlook

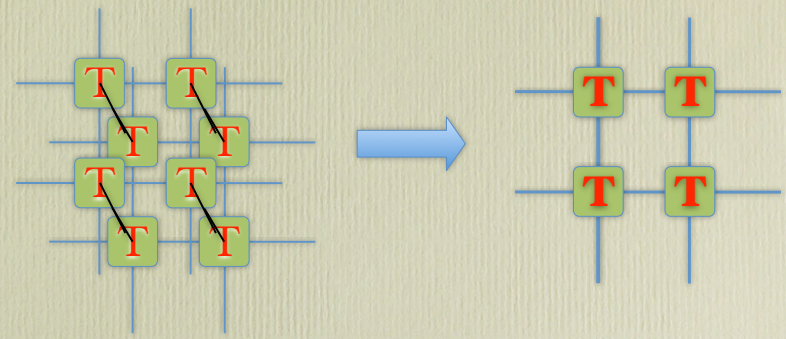
- Application of TPS/TRG to bosonic system
- Two-Species Bose-Hubbard Model
  - Phase diagram
  - Paired SuperFluid
- Improve the accuracy
  - Improved optimization and contraction method
  - SRG, CTMRG, etc

Thank You
ありがとう

謝謝

Expectation Value of TPS

$\langle \Psi | \Psi \rangle =$



Double tensor **T**

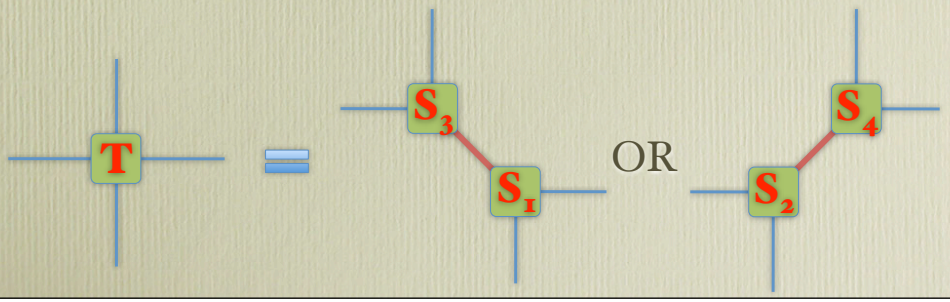
$$\mathbf{T}_{(\tilde{u}u\tilde{l}l\tilde{d}d\tilde{r}r)} = \sum_{S} T^{*S}_{\tilde{u}\tilde{l}\tilde{d}\tilde{r}} T^{S}_{uldr}$$

$$\mathbf{T}^{A}_{(\tilde{u}u\tilde{l}l\tilde{d}d\tilde{r}r)} = \sum_{\tilde{S}S} T^{*\tilde{S}}_{\tilde{u}\tilde{l}\tilde{d}\tilde{r}} \langle \tilde{S} | O^{A} | S \rangle T^{S}_{uldr}$$

Tensor Renormalization Group

Rewrite rank 4 tensor **T** into product of two rank 3 tensor **S**

$$\mathbf{T}_{\alpha\beta\mu\nu} \cong \sum_{\gamma=1}^{D_{cut}} S_{3,\alpha\delta\gamma} S_{1,\mu\nu\gamma}$$



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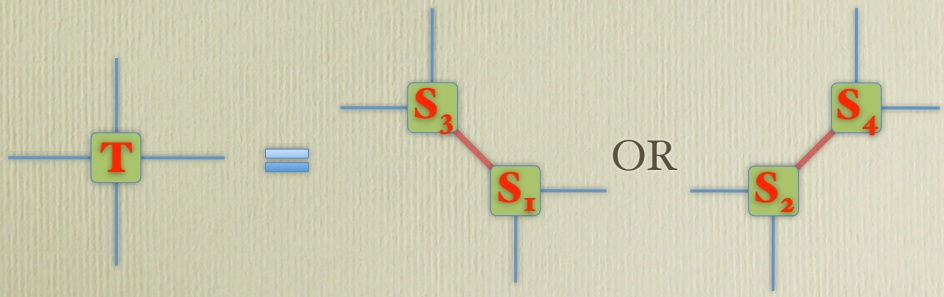

- M. Levin and C. P. Nave, Phys. Rev. Lett. 99, 120601, 2007
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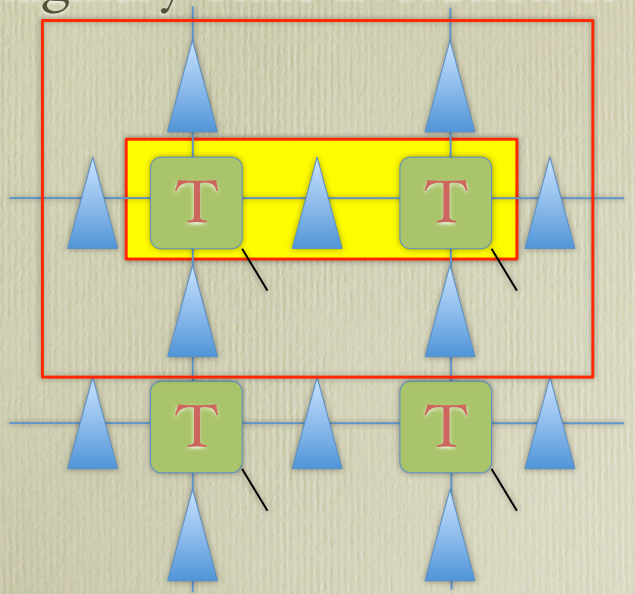
Imaginary Time Evolution of TPS



- H. C. Jiang, Z. Y. Weng, and T. Xiang, Phys. Rev. Lett. 101,090603 ,2008
- Z. Y. Xie, H. C. Jiang, Q. N. Chen, Z. Y. Weng, and T. Xiang, Phys. Rev. Lett. 103, 160601,2009