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Contractor Renormalization for Strongly Correlated Electrons

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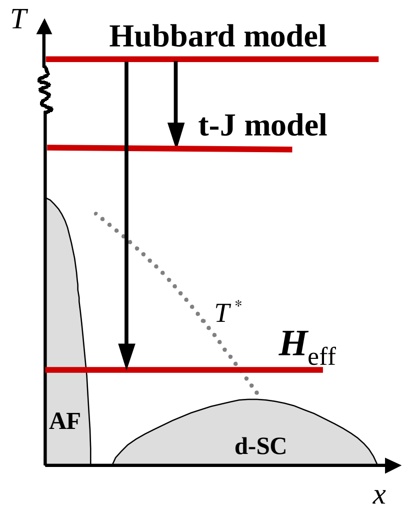
Outline

1. **Renormalization and Effective Hamiltonians**
2. **Contractor Renormalization**
3. **2-D Hubbard =>** Plaquette Boson-Fermion Model
4. **Quantum Frustration: Checkerboard and Pyrochlore lattices**

References:
Cuprates:
E. Altman and A. Auerbach, ***Phys. Rev. B65, 104508, 2002.***

Pyrochlores: E. Berg, E. Altman and A. Auerbach, ***cond-mat/0206384; PRL submitted.***

The Cuprate Problem



Effective Hamiltonian which includes:

1. Tightly bound d-wave pairs
2. Antiferromagnetic correlations

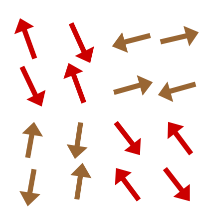
Can we get this from a strong repulsively interacting electrons model ?

Problem: Quantum Frustration

$$H = J\sum_{\langle ij\rangle} \mathbf{S}_i \cdot \mathbf{S}_j = J\sum_{tet} \mathbf{S}_{tet}^2 + const$$

Pyrochlore

Checkerboard

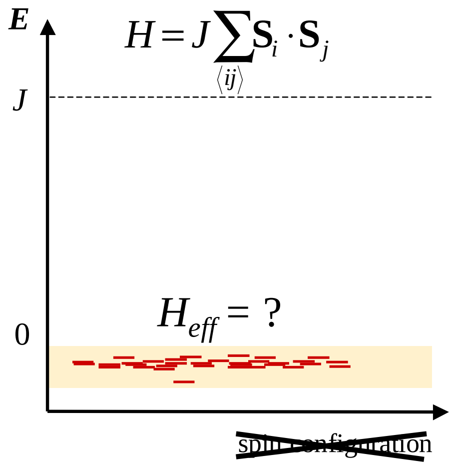


Extensive number (N/2) degrees of freedom in classical GS manifold

Spinwave theory is poorly controlled

Highly frustrated magnets

Checkerboard



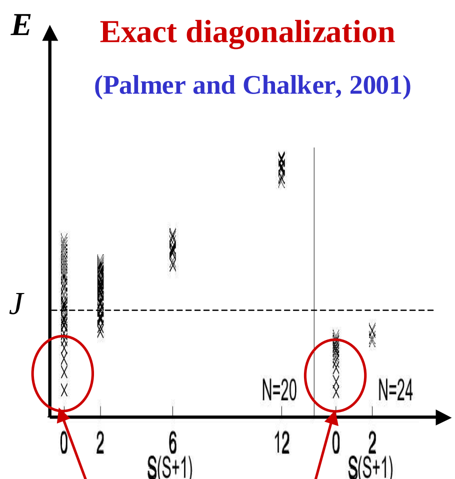
Pyrochlore

Strong Quantum fluctuations (spin-½) ?

Spin-½ Checkerboard Antiferromagnet

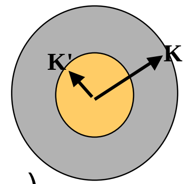
Exact diagonalization

(Palmer and Chalker, 2001)



How to describe ground state and low energy singlets ?

k-Space Renormalization (Shankar)

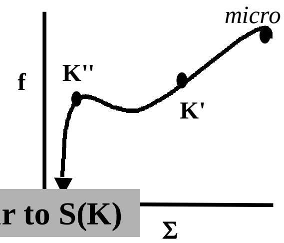


Eliminate high momenta single particle states

$$Z_{micro} = \int D^2 z \, \boldsymbol{exp}\left(- \int d\tau \bar{z} \partial_\tau z - H[\bar{z}, z] \right)$$
$$= \int D^2 z_{k<K'} \, \boldsymbol{exp}\left(- S[z(\tau'), \tau] \right)$$

$$S_{K'} \approx \sum_{k<K'} \left(i\omega - \varepsilon_k - \Sigma(k,\omega) \right) \bar{z}_k z_k - f \, \bar{z}_k \bar{z}_{k'} z_{k''} z_{k+k'-k''} + \dots$$

"Effective Hamiltonian"



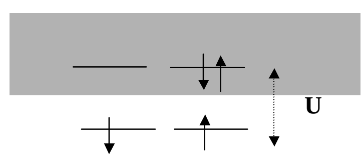
Renormalization group: S(K)--> S(K')

Couplings flow: f(K), Σ(K)

Provision: S(K') should be similar to S(K)

Renormalization by Cannonical Transformation

$$H = -t \sum_{ij} c_{is}^{+} c_{js} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$



Schrieffer-Wolff -> $H^{eff} \approx \frac{4t^2}{U} \sum_{ij} S_i \cdot S_j + O(t/U, E/U)$

$\vec{S} = \frac{1}{2} c_s^{+} \vec{\sigma}_{ss'} c_{s'}$

Advantages

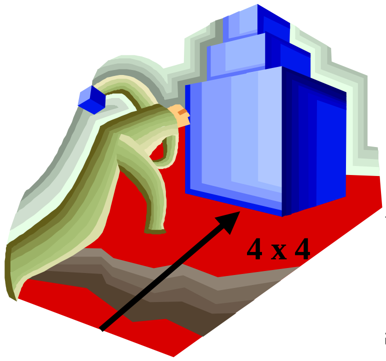
1. Reduced Hilbert Space
2. Bosonic degrees of freedom
3. Better mean field approximations for Heisenberg than for the Hubbard Model (large S, Large N)

Problems:

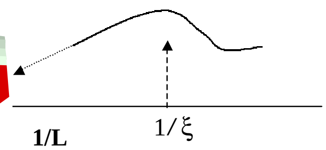
(1) Pertubative limit of (t/U)<<1

(2) H(E) is not *really* a Hamiltonian

Direct Numerical Correlations



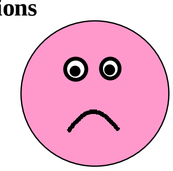
Need $L > \xi_{\text{correlation}}$



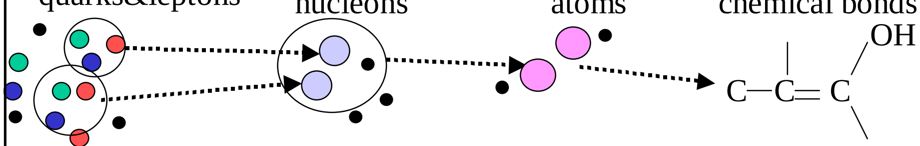
ation time is $\approx exp\left(L^d\right)$

If ξ is large, it is futile to try to extract thermodynamic correlations

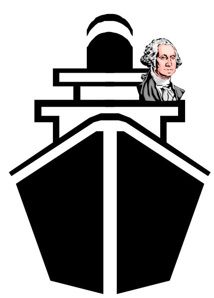
What are numerics good for?



Emerging Low Energy Degrees of Freedom

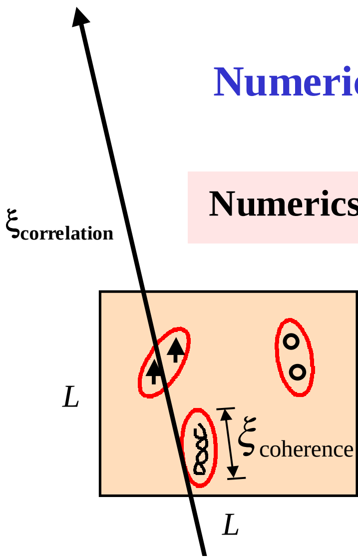


The Captain's Weight



Numerical Renormalization

Numerics ⟶ $H_{effective}$



Need only $L > \xi_{\text{coherence}}$ **!**

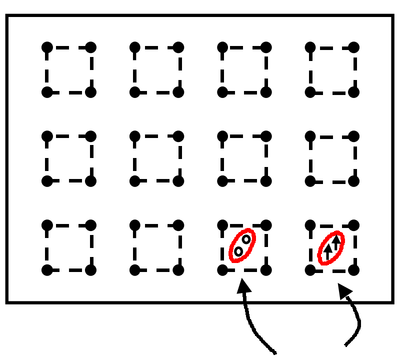
$\xi_{\text{coherence}}$ **= size of “atoms”**

How do we identify “atoms” and calculate effective couplings??

Contractor Renormalization (CORE)

Morningstar-Weinstein, PRD (1996)

Step I: Divide lattice to disjoint blocks



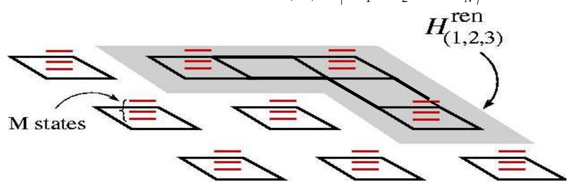
“atoms”

Truncate:

$N \rightarrow M$ **lowest states per block** $\{|\phi_i\rangle\}_{i=1}^{M}$

Step II: H^{ren} for a particular cluster of N blocks

Reduced Hilbert space: $|\alpha\rangle = |\phi_{i_1}, \phi_{i_2} \ldots \phi_{i_N}\rangle$ (dim= M^N)



3. Orthonormalize from ground state up. (Gramm-Schmidt)

$$\varepsilon_n \;, \; |n\rangle, \; \sum P_\alpha |n\rangle \longrightarrow |\psi_n\rangle$$

$$|\tilde{\psi}_n\rangle = \frac{1}{Z_n}\left(|\psi_n\rangle - \sum_{m<n} |\tilde{\psi}_m\rangle \langle \tilde{\psi}_m | \psi_n \rangle \right)$$

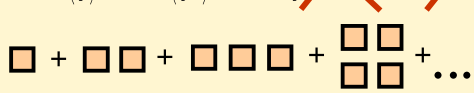
$$H^{ren}_{(1,\ldots,N)} \equiv \sum_{n=1}^{M^N} \varepsilon_n |\tilde{\psi}_n\rangle\langle\tilde{\psi}_n|$$

$$h_{(1,\ldots N)} \equiv H^{ren}_{(1,\ldots,N)} - \sum_{i_1,\ldots i_L}^{conn.subclus.} h_{i_1,\ldots i_L}$$

Step III: Cluster Expansion

2. CORE Exact Identity:

$$H_{eff} = \sum_i h_i + \sum_{\langle ij \rangle} h_{ij} + \sum_{\langle ijk \rangle} h_{ijk} + \sum_{ijk\ldots} h_{ijk\ldots} \cdots$$



3. Truncate at finite range

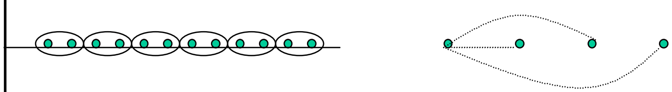
truncation error?

A short emerging length scale $\xi_{\text{coherence}}$ controls expansion

Test: 1D Heisenberg

S=1/2 Heisenberg chain

$$JS_i \cdot S_{i+1} \longrightarrow E_0 / N = \sum_r h_0^r$$



C.J. Morningstar&M. Weinstein hep-lat/000202

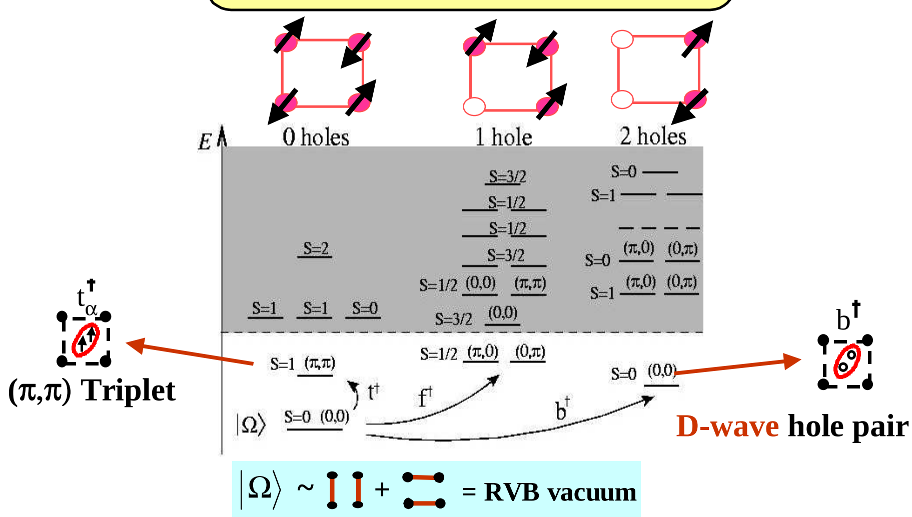
Table 1: Spin-1/2 HAF: Exact Energy Density $= -\ln(2) + 1/4 = -0.4431472$

Range (sites)	Energy Density CORE	Padé [N/M]	Energy Density
1 (2)	-0.3750000		
2 (4)	-0.4330127		
3 (6)	-0.4387759	[1/1]	-0.4428182
4 (8)	-0.4406777	[1/2]	-0.4431005
		[2/1]	-0.4431022
5 (10)	-0.44155130	[2/2]	-0.4431337
6 (12)	-0.44202771	[2/3]	-0.4431412
		[3/2]	-0.4431412

Heisenberg Ladders: Piekarewicz and Shepard,(1997)

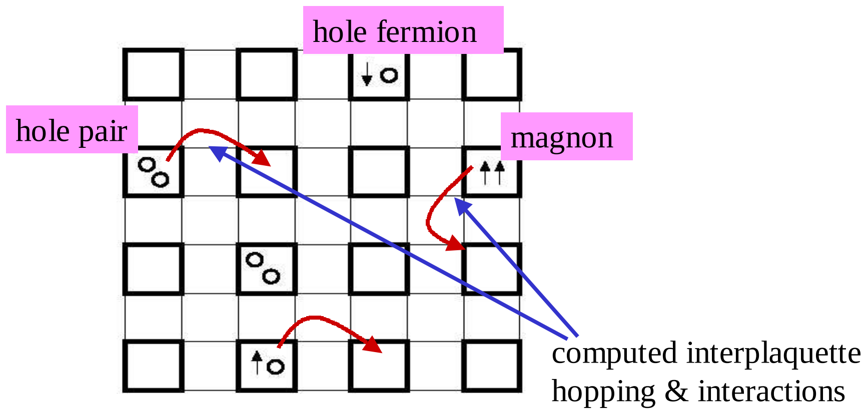
Altman & A.A., (2001), Poilblanc & Capponi, *preprint.*

Hubbard Plaquette States



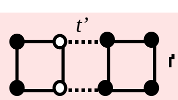
AFmagnet and Superconductor degrees of freedom !

Coupling Plaquettes (CORE)



"*Plaquette Boson Fermion Model of Cuprates*"
E. Altman and A.A., *Phys. Rev. B65, 104508 2002.*

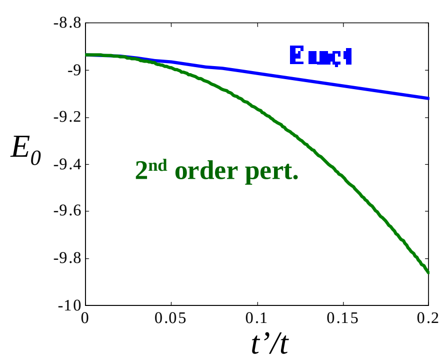
Coupling plaquettes:
Failure of perturbative approach



Pair hopping: $J_C \propto \frac{t'^2}{\Delta_b}$

Fails for $t' > \Delta_b$

Energy of 2 holes on the cluster

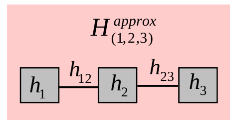


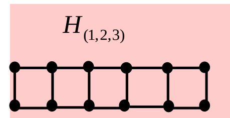
Good convergence of the cluster expansion!

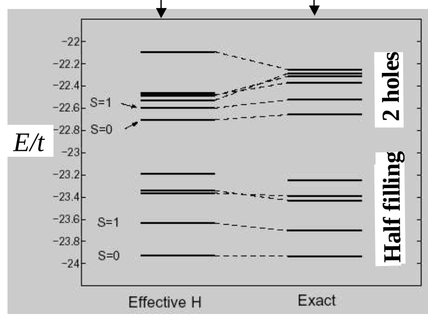
$$\langle h_{ijk} \rangle / \langle h_{ij} \rangle \sim 10^{-1} - 10^{-2}$$

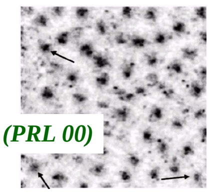
$$\Downarrow$$

Short coherence length!







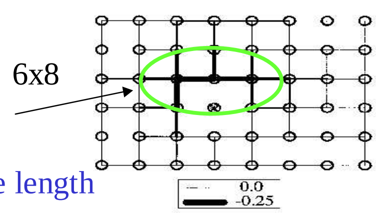


S.H. Pan etal (PRL 00)

Pairs keep their integrity on the full lattice!!

Pair Integrity

Pair correlations in t-J model by DMRG (*White&Scalapino*)

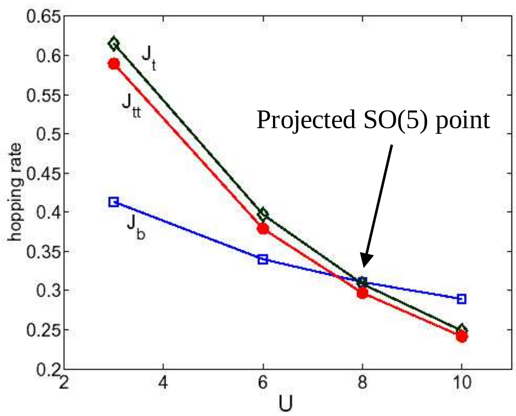


Hole pairs stay tightly bound in larger clusters

Four Boson Model

$$\mathcal{H}^b = (\epsilon_b - 2\mu)\sum_i b_i^\dagger b_i - J_b \sum_{\langle ij\rangle}\left(b_i^\dagger b_j + \text{H.c.}\right)$$

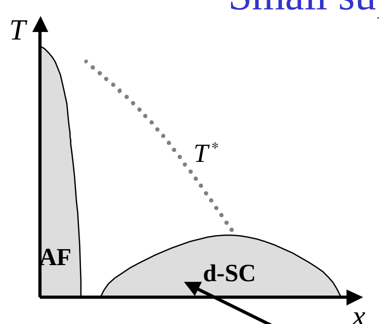
$$\mathcal{H}^t = \epsilon_t \sum_{i\alpha} t_{\alpha i}^\dagger t_{\alpha i} - \frac{J_t}{2}\sum_{\alpha\langle ij\rangle}(t_{\alpha i}^\dagger t_{\alpha j} + \text{H.c.}) - \frac{J_{tt}}{2}\sum_{\alpha\langle ij\rangle}(t_{\alpha i}^\dagger t_{\alpha j}^\dagger + \text{H.c.})$$



Projected SO(5) Theory
S-C Zhang, J.P. Hu, E. Arrigoni, W. Hanke, A. Auerbach, PRB60, (99)
Numerics:
Dorneich, Hanke,Arrigoni, Troyer, Zhang,(02)

Similar scale for pair and magnon hopping!

Small superfluid density

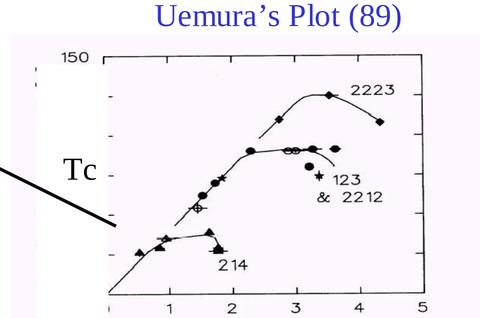


$$H = \tfrac{1}{2}\rho_c \int d^2x \left((\nabla + iA)\varphi\right)^2$$

Ginzburg-Landau

$$\rho_c \propto 1/\lambda^2$$

Uemura's Plot (89)



$$\rho_c \propto 1 - n_e$$

BEC of real-space pairs

BCS

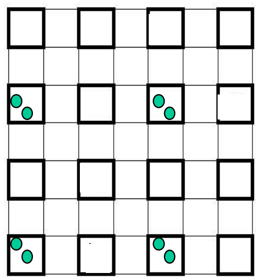
$\rho_c \approx \hbar^2 n_e / 2m \approx \varepsilon_F \approx 1eV$

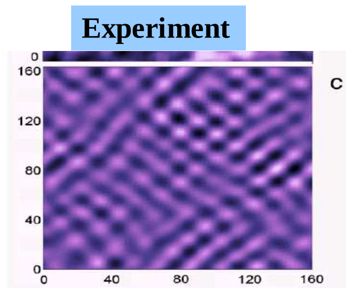
$T_c \approx \omega_D e^{-1/\lambda} \approx 10^{-3} eV$

$n_e \approx 1/a^2$

T_c, ρ_c, n_e unrelated

Plaquettized Lattice?





Howland etal (02)

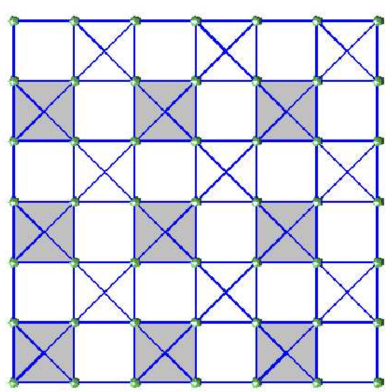
x=0.125
condensate wave $\langle b_r \rangle \propto e^{iQr}$
Q= $(\pi/2, 0)+(0,\pi/2)$

Modulation of period 4 in tunneling conductance

Stripes,

or Plaquettized order parameter?

Back to the Pyrochlores:

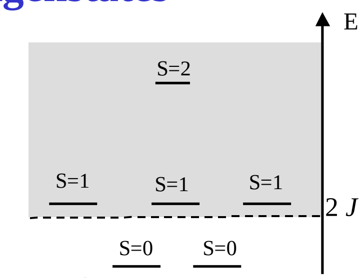


back

Goal: H_{eff} **in terms of lowest tetrahedron states**

Tetrahedron eigenstates

$$H(\boxtimes) = JS_{tot}^2 + c$$



Pseudospin Variable:

$$— = \tfrac{1}{\sqrt{2}}(\uparrow\downarrow - \downarrow\uparrow)$$

$$|\Rightarrow\rangle = \tfrac{1}{\sqrt{3}}(\boxtimes + \boxtimes)$$

$$|\Leftrightarrow\rangle = \boxtimes - \boxtimes$$

Effective Hamiltonian

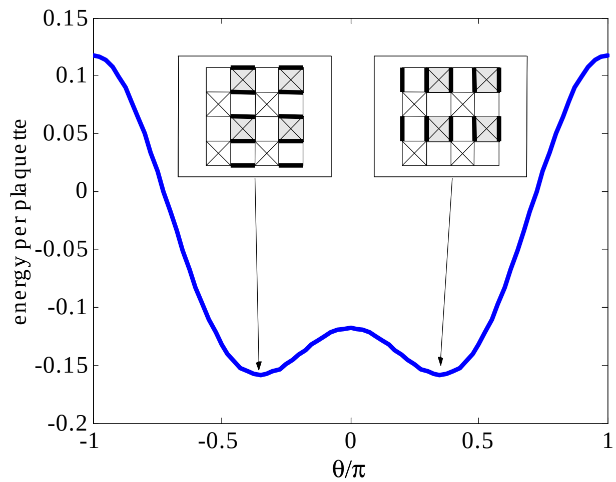
$$H_{eff} = \sum_i h_i(\boxtimes) + \sum_{ij} h_{ij}(\boxtimes\boxtimes) + \sum_{ijk} h_{ijk}(\boxtimes\boxtimes\boxtimes) + \sum_{ijkl} h_{ijkl}(\boxtimes\boxtimes\boxtimes\boxtimes) + \ldots$$

$$\Rightarrow H_{eff} = -J_I \sum_{\langle ij \rangle} (\bar{S}_i \cdot \hat{\Omega}_{ij})(\bar{S}_j \cdot \hat{\Omega}_{ij}) - h_I \sum_i S_i^z$$

$$J_I \cong J/2$$
$$h_I \cong J/4$$

$$\hat{\Omega}_{Verticle} = \nwarrow \qquad \hat{\Omega}_{Horizontal} = \nearrow$$

Mean Field solution



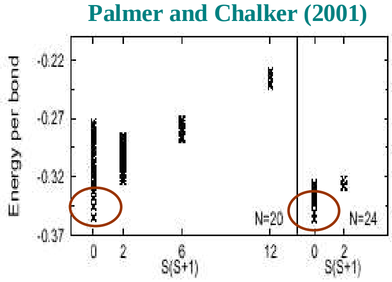
Direction of pseudospins

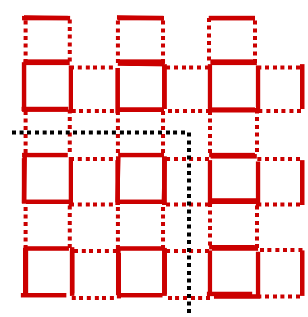
Thermodynamics

Crossed plaquettes are symmetric with respect to the degenerate ground states!

Singlet Excitations
↕
Ising Domain walls

Palmer and Chalker (2001)





H_{eff}

⇓

Spin flip excitation energy ~ J/2

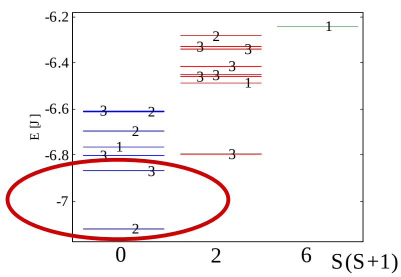
Number of low singlet excitation grows linearly with size

Quantum Pyrochlore Antiferromagnet

No MF order down to zero temperature!

Villain (79);
Moessner and Chalker (98);

Spectrum of a finite cluster of the spin-½ Pyrochlore



First CORE Step

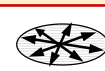
First stage: Tetrahedral clustering

Pseudospins defined on a FCC lattice

Effective 3-body hamiltonian

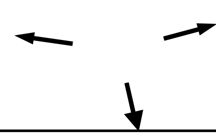
$$H_{eff} \approx J_3 \sum_{\langle ij \rangle} \left(\frac{1}{2} + \bar{S}_i \cdot \bar{e}_{ijk} \right) \left(\frac{1}{2} + \bar{S}_j \cdot \bar{e}_{ijk} \right) \left(\frac{1}{2} + \bar{S}_k \cdot \bar{e}_{ijk} \right)$$

Perturbative Expansion: Harris, Berlinsky,Bruder (92)



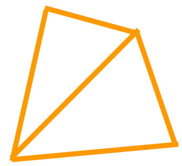
MF level: four sublattice "Order"

Remaining macroscopic degeneracy!

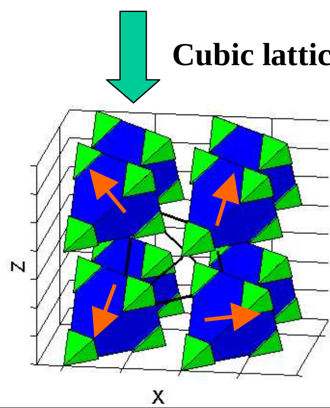


Second CORE step

Second stage: "Super Tetrahedral" clustering

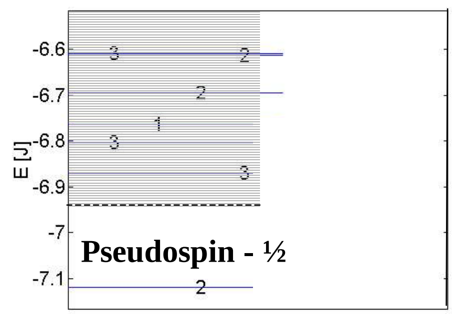


Cubic lattice



Basic block: "supertetrahedron"

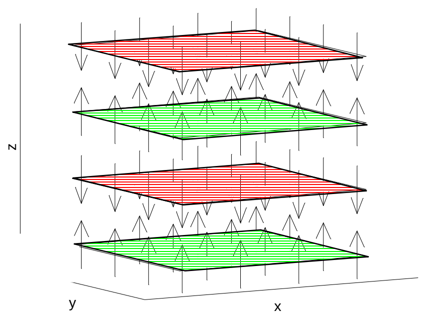
Spectrum of a single block:



Mean Field Solution

$$H_{eff} = J_a \sum_{\langle ij \rangle} \left(\vec{S}_i \cdot \vec{e}_{ij}\right)\left(\vec{S}_j \cdot \vec{e}_{ij}\right) + J_b \sum_{\langle\langle ij \rangle\rangle} \left(\vec{S}_i \cdot \vec{e}_{ij}\right)\left(\vec{S}_j \cdot \vec{e}_{ij}\right) + \ldots$$

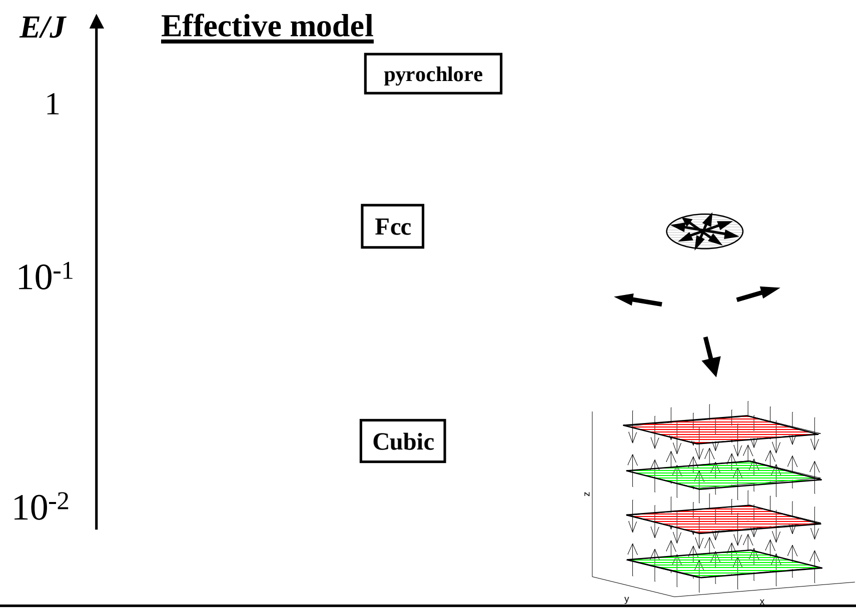
Mean field ground state:



Supertetrahedron pseudospins

- **Ground state: 6 fold degeneracy, rotational and translational symmetry breaking**
- **Coherence length: ~ single supertetrahedron**
- **Domain wall excitations**

Energy Scale of the effective couplings



Summary

1. **CORE renormalizes a microscopic Hamiltonian to an effective <u>Hamiltonian</u>, non perturbatively.**

2. **The truncation error can be controlled by a short coherence length (``*atom size*'').**

3. Applying CORE to the Hubbard Model yields an effective Plaquette Boson Fermion Model.

4. Applying CORE to the Pyrochlore yields a lattice symmetry breaking ground state and very low lying singlet excitations.

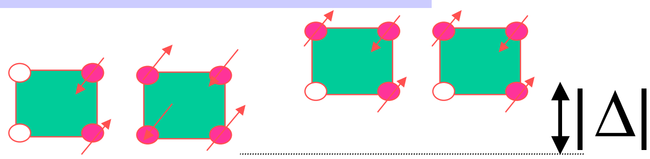
<u>Future:</u>

Development of larger scale CORE computations (S. Capponi)

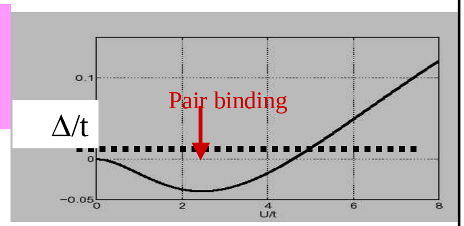
Explore the PBFM.

Pair Binding on a Plaquette

$$\Delta \equiv E_2 - 2E_3 + E_4 < 0$$

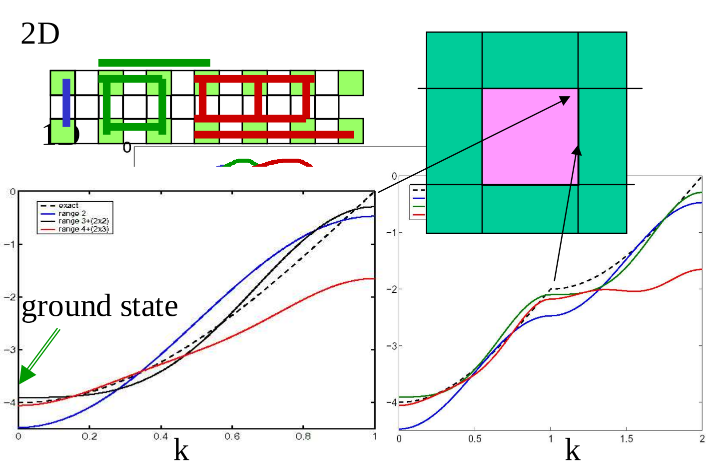


Pair binding was found for Hubbard and t-J clusters close to half filling!
(Hirsch et.al., Fye et.al 89.)



Is this the Pairing Mechanism?

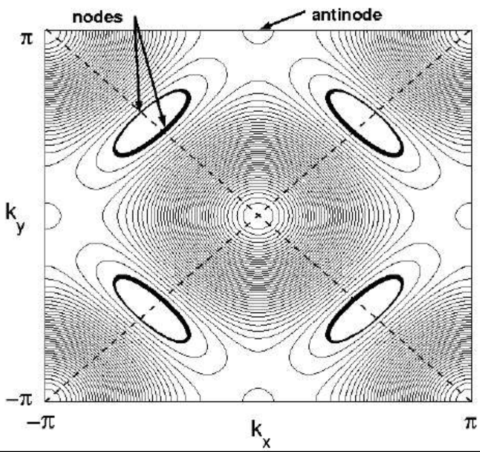
Test: Tight Binding models



Fermion holes

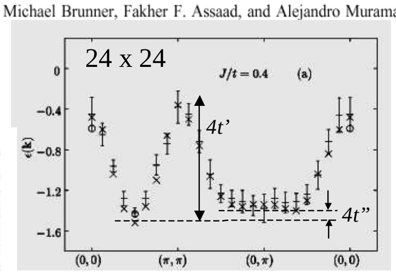
$$\mathcal{H}^f = \sum_{\mathbf{k}s} (\epsilon^f_{\mathbf{k}} - \mu) f^\dagger_{\mathbf{k}s} f_{\mathbf{k}s}$$

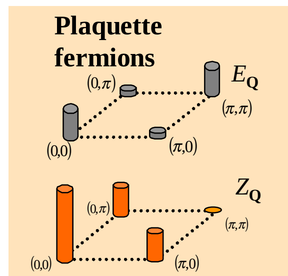
$$\varepsilon_{\mathbf{k}} \approx t'(\cos k_x + \cos k_y)^2 + t''(\cos k_x - \cos k_y)^2$$



Single-hole dynamics in the *t*-*J* model on a square lattice

Michael Brunner, Fakher F. Assaad, and Alejandro Muramatsu





VOLUME 81, NUMBER 14 PHYSICAL REVIEW LETTERS 5 OCTOBER 1998

Violation of Luttinger's Theorem in the Two-Dimensional *t*-*J* Model

W. O. Putikka,[1,2] M. U. Luchini,[3,4] and R. R. P. Singh[5]

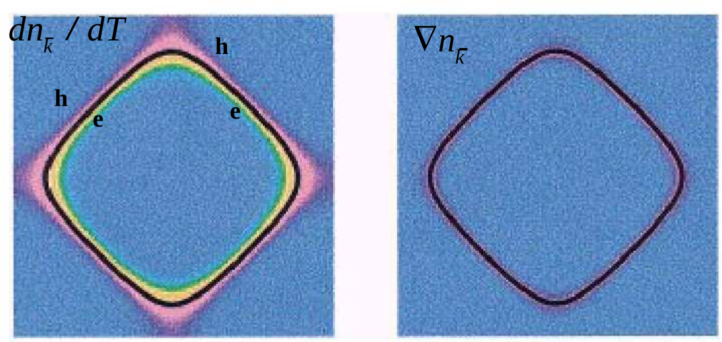
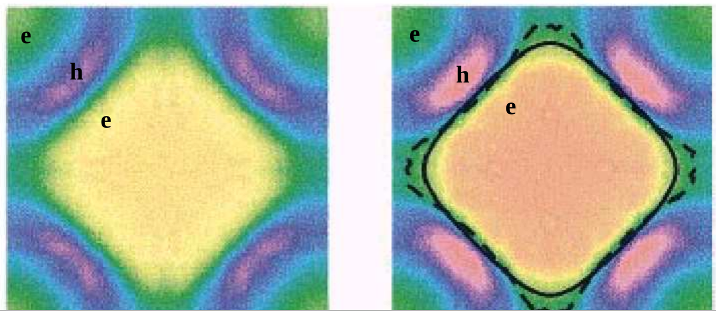


FIG. 3(color). Full Brillouin zone plots for the tight-binding model at $n = 0.80$. Left: $\Delta n_{\mathbf{k}}/\Delta T$ for $\bar{T} = 0.3J = 0.12t$;

Non Interacting, Tight Binding

$dn_{\bar{k}} / dT \quad (T = 0.5J)$ $\qquad$ $dn_{\bar{k}} / dT \quad (T = 0.3J)$



t-J Model

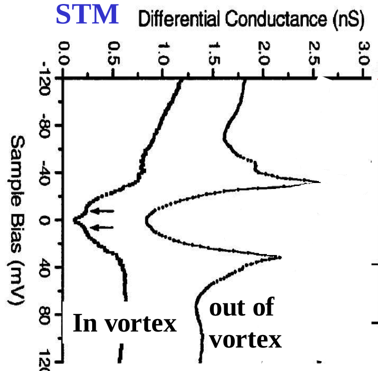
FIG. 4(color). Full Brillouin zone plots of $\Delta n_{\mathbf{k}}/\Delta T$ for the t-J model. The color scale is the same for both plots. Orange, yellow, and green are negative, with a minimum value of $\Delta n_{\mathbf{k}}/\Delta T = -0.08J^{-1}$. Blue, violet, and red are positive, with a maximum value of $\Delta n_{\mathbf{k}}/\Delta T = 0.15J^{-1}$. The plots correspond to different temperatures; left: $\bar{T} = 0.5J$; right: $\bar{T} = 0.3J$. In the right plot the solid curve is the $T = 0$ tight-

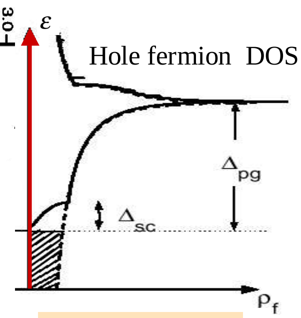
Plaquette Boson – Fermion Model

$$H^{PBFM} = H^{bosons} + H^{fermions} + H^{bf}$$

$$\mathcal{H}^{bf} = g_b \sum_{\mathbf{k},\mathbf{q}} \left(d_{\mathbf{k}+\mathbf{q}/2} b^{\dagger}_{\mathbf{q}} f_{\mathbf{k}\uparrow} f_{-\mathbf{k}+\mathbf{q}\downarrow} + \text{H.c} \right)$$

STM





Hole fermions at $\mathbf{q} \approx \left(\pm \frac{\pi}{2}, \pm \frac{\pi}{2}\right)$

Pseudogap

$\Delta^{pg} \cong E_{\mathbf{k}^{sp}} - \mu(x,T)$

$\mu(x) - \mu(0) = \dfrac{x}{(2\kappa_b + \kappa_f)}$

Superconducting gap

$\Delta^{sc}_{\mathbf{k}} = g_b d_{\mathbf{k}} \langle b \rangle$

$E_k = \sqrt{(\varepsilon_{\mathbf{k}} - \mu)^2 + (\Delta^{SC}_{\mathbf{k}})^2}$

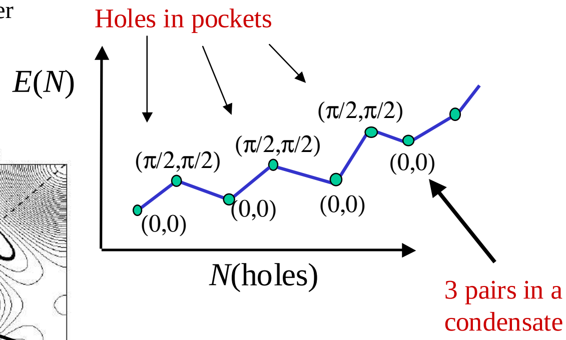
S.H. Pan etal (PRL 00)

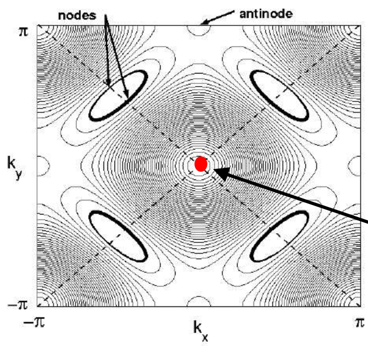
Numerical support

Static and dynamical properties of doped Hubbard clusters

E. Dagotto, A. Moreo, F. Ortolani,* D. Poilblanc,† and J. Riera‡

4X4 cluster





Pair condensate

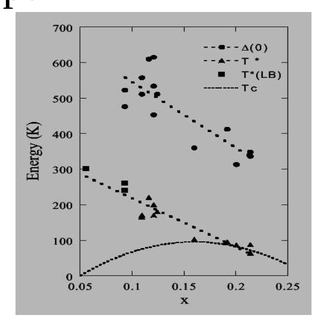
The problem of Two Gaps

Pseudogap **decreases** with doping
(measures chemical potential)

$$\mu(x) - \mu(0) = \frac{x}{(2\kappa_b + \kappa_f)}$$

$$\Delta^{pg} \cong E_{\mathbf{k}^{sp}} - \mu(x,T)$$

Coherence gap **increases** with doping
(measures hole pairs order parameter)



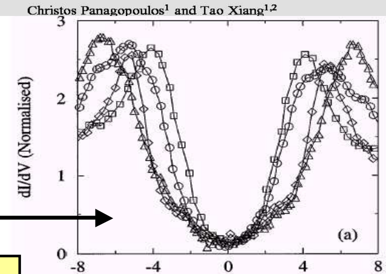
Relationship between the Superconducting Energy Gap and the Critical Temperature in High-T_c Superconductors

Christos Panagopoulos[1] and Tao Xiang[1,2]

Tunneling:

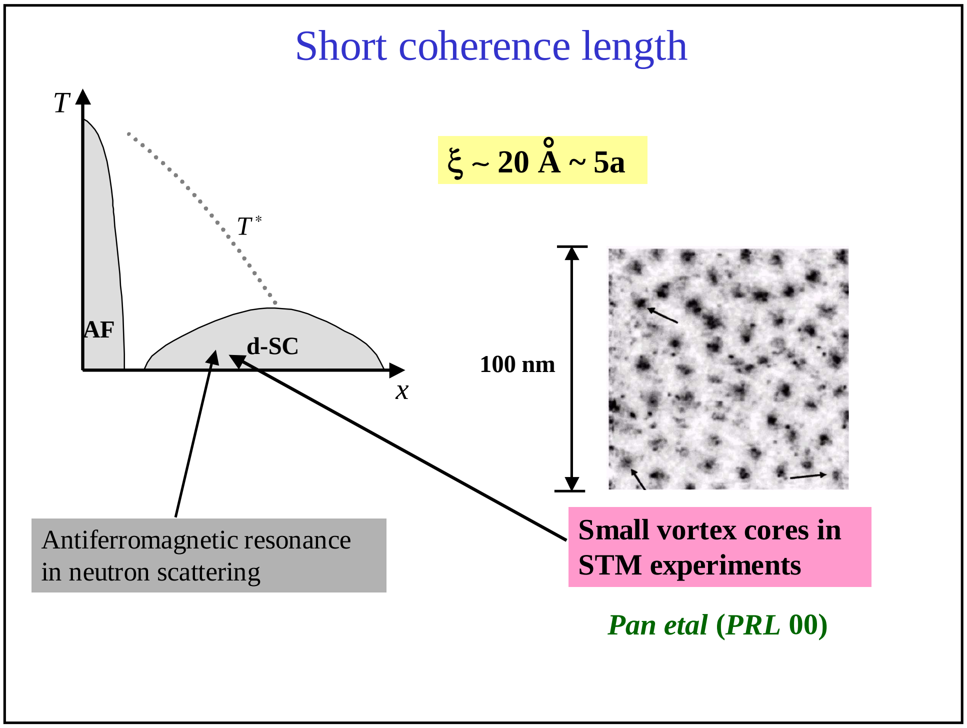
$$\mathcal{H}^{bf} = g_b \sum_{\mathbf{k},\mathbf{q}} \left(d_{\mathbf{k}+\mathbf{q}/2} b^\dagger_{\mathbf{q}} f_{\mathbf{k}\uparrow} f_{-\mathbf{k}+\mathbf{q}\downarrow} + \mathrm{H.c} \right)$$

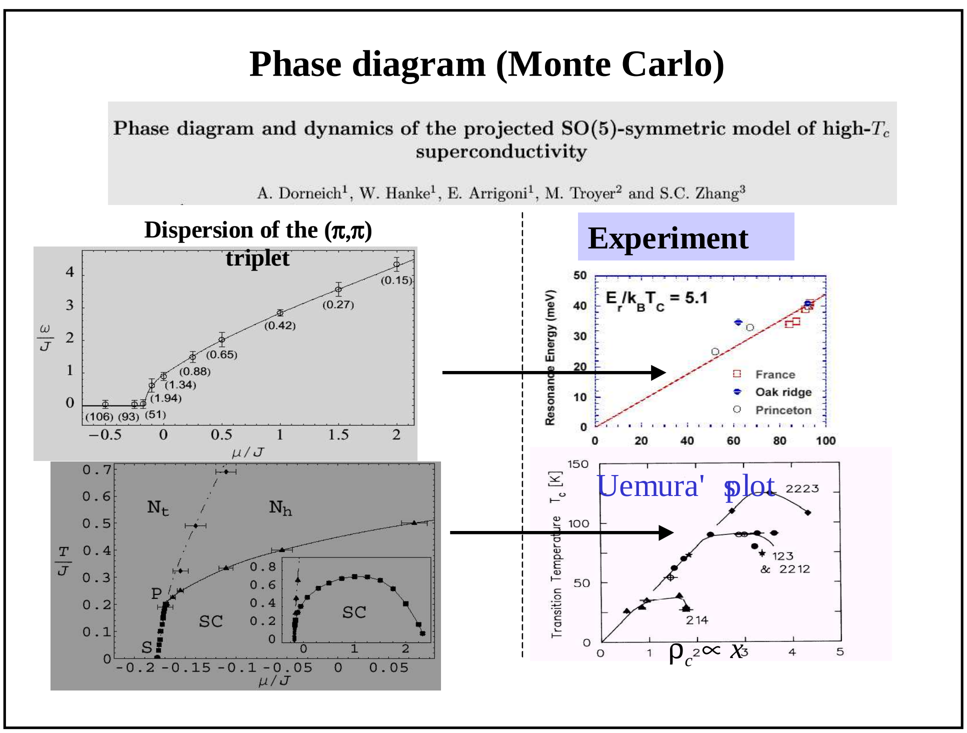
$$\Delta^{sc}_{\mathbf{k}} = g_b d_{\mathbf{k}} \langle b \rangle$$



pseudogap

Prediction: $\Delta_{SC} \propto \sqrt{T_C}$


Short coherence length
T
ξ ~ 20 Å ~ 5a
T*
AF
d-SC
x
100 nm
Antiferromagnetic resonance in neutron scattering
Small vortex cores in STM experiments
Pan etal (PRL 00)


Phase diagram (Monte Carlo)
Phase diagram and dynamics of the projected SO(5)-symmetric model of high-T_c superconductivity
A. Dorneich[1], W. Hanke[1], E. Arrigoni[1], M. Troyer[2] and S.C. Zhang[3]
Dispersion of the (π,π) triplet
Experiment
E_r/k_BT_c = 5.1
France
Oak ridge
Princeton
Resonance Energy (meV)
Uemura' plot
$\rho_c^2 \propto x$
Transition Temperature T_c [K]
2223
123 & 2212
214
N_t
N_h
P
SC
S
μ/J
T/J
ω/J

$$h_{ijk} \approx J_3\left(\frac{1}{2}+\bar{S}_j\cdot\bar{e}_{ijk}\right)\left(\frac{1}{2}+\bar{S}_j\cdot\bar{e}_{ijk}\right)\left(\frac{1}{2}+\bar{S}_k\cdot\bar{e}_{ijk}\right)$$