Computational Approaches to
Quantum Critical Phenomena
(2006.7.17-8.11) ISSP

Fermion Simulations

July 31, 2006

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ISSP, Kashiwa

collaboration

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Numerical Methods for Lattice Fermions

exact diagonalization	small clusters
high-temperature expansion	high to moderate T
DMRG	1D systems
variational Monte Carlo	trial wave functions
cellular (cluster) DMFT	small cluster + DMF
quantum Monte Carlo	negative sign
auxiliary field	
world line	
PIRG	
Gaussian basis	

PIRG: nonperturbative but systematic approach from U=0

the only available approach for frustrated models,
complex systems with orbital at T=0 for large size

Path-Integral Representation

$$|\Phi\rangle = \lim_{p\to\infty}[\exp[-\Delta_\beta H]]^p |\Phi_0\rangle$$

Practically, taking small Δ_β, but $\Delta_\beta p$ large

$$|\Phi'\rangle = \exp[-\Delta_\beta H]|\Phi\rangle$$

$$\approx \exp[-\Delta_\beta H_0/2]\exp[-\Delta_\beta H_1]\exp[-\Delta_\beta H_0/2]|\Phi\rangle + O(\Delta_\beta{}^3)$$

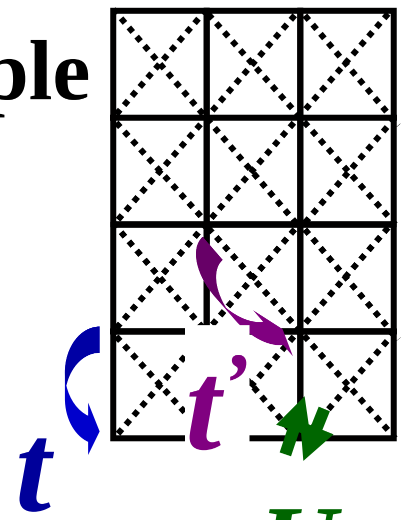
Hubbard model

$$H = H_0 + H_1$$

$$H_0 = \sum_{ij\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \mathrm{H.c}$$

$$H_1 = U \sum n_{i\downarrow} n_{i\uparrow}$$

example



Matrix representation of Slater determinant $|\Phi\rangle$

M Fermions on *N*-sites lattice

$$|\Phi_\sigma\rangle = \prod_{m=1}^{M} \Big(\sum_{i=1}^{N} (\Phi_\sigma)_{im} c_{i\sigma}^\dagger\Big)|0\rangle$$

$$N \left\{ \underbrace{\begin{pmatrix} (\Phi_\sigma)_{im} & \\ & \\ & \end{pmatrix}}_{M} \right.$$

inner product

$$\langle\Phi_\sigma|\Phi'_\sigma\rangle = \det({}^t\Phi_\sigma \Phi'_\sigma)$$

Example; plane wave state

$$\sum_{i=1}^{N} \cos(\mathbf{k}_n \cdot \mathbf{r}_i) c_i^\dagger |0\rangle$$

$$\sum_{i=1}^{N} \sin(\mathbf{k}_n \cdot \mathbf{r}_i) c_i^\dagger |0\rangle$$

$$\begin{aligned} \Phi_{i,2n-1} &= \cos(\mathbf{k}_n \cdot \mathbf{r}_i), \\ \Phi_{i,2n} &= \sin(\mathbf{k}_n \cdot \mathbf{r}_i) \end{aligned}$$

SDW Hartree-Fock State

$$\Phi_{\sigma i,2n-1} = \sqrt{\frac{1-d_{k_n}}{2}}\cos(\mathbf{k}_n\cdot\mathbf{r}_i) \pm\sqrt{\frac{1-d_{k_n}}{2}}\cos((\mathbf{k}_n+\mathbf{k}_s)\cdot\mathbf{r}_i)$$

$$\Phi_{\sigma i,2n} = \sqrt{\frac{1-d_{k_n}}{2}}\sin(\mathbf{k}_n\cdot\mathbf{r}_i) \pm\sqrt{\frac{1-d_{k_n}}{2}}\sin((\mathbf{k}_n+\mathbf{k}_s)\cdot\mathbf{r}_i),$$

$$d_k = \frac{E_k}{\sqrt{\Delta_s^2+E_k^2}}$$

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Operation of Kinetic Energy Projection

$$|\Phi'\rangle = \exp[-\Delta_\beta H_0]|\Phi\rangle$$

bilinear tight-binding form

$$H_0 = \Sigma\,[t_{ij}\, c^\dagger_{i\sigma} c_{j\sigma} + \mathrm{H.c} + \delta_{ij}\mu\, c^\dagger_{i\sigma} c_{j\sigma}\,]$$

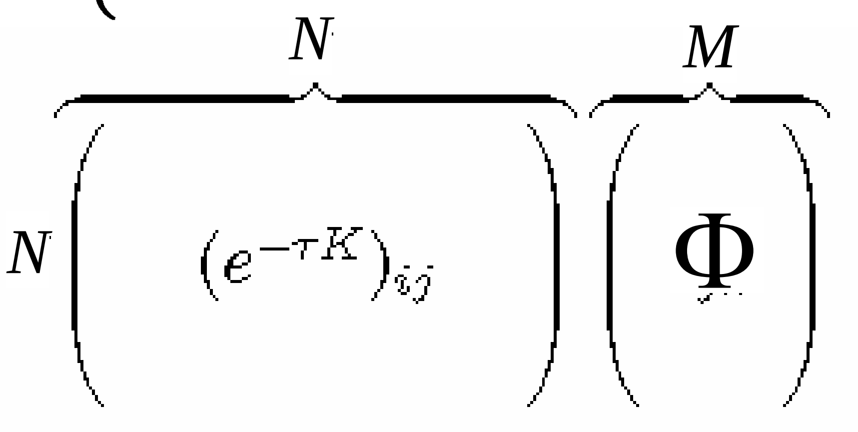
Matrix representation

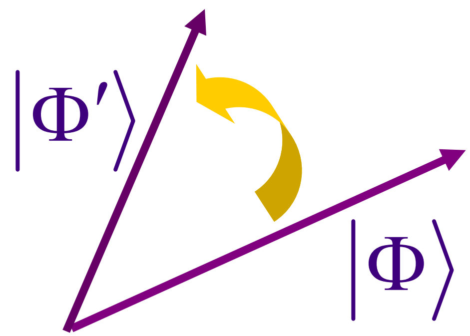
of $\exp[-\Delta_\beta H_0] \Rightarrow b_0$

In Slater determinant representation, exponential of kinetic energy generates another Slater deteremeinants

$$b_0 = \exp[-K]$$

$$K_{ij} = \begin{cases} -\Delta_\beta t & \text{if } (i,j) \text{ is the nearest neighbor} \\ = 0 & \text{otherwise} \end{cases}$$





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Operation of Coulomb Energy Projection

$$|\Phi'\rangle = \exp[-\Delta_\beta H_1]|\Phi\rangle \ ??$$

$$H_1 = U\sum c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow}$$

Projection by the interaction term
is transformed to a sum of
two Slater determinants
by Stratonovich-Hubbard transformation

Stratonovich-Hubbard Transformation

Discrete transformation

Auxiliary Ising variable *s*

$$e^{-\alpha n_\uparrow n_\downarrow} = \frac{1}{2}\sum_{s=\pm 1} \exp[2as(n_\uparrow - n_\downarrow) - \frac{\alpha}{2}(n_\uparrow + n_\downarrow)]$$

$$a = \mathrm{th}^{-1}\sqrt{\mathrm{th}(\frac{\alpha}{4})} \qquad (1)$$

decomposition

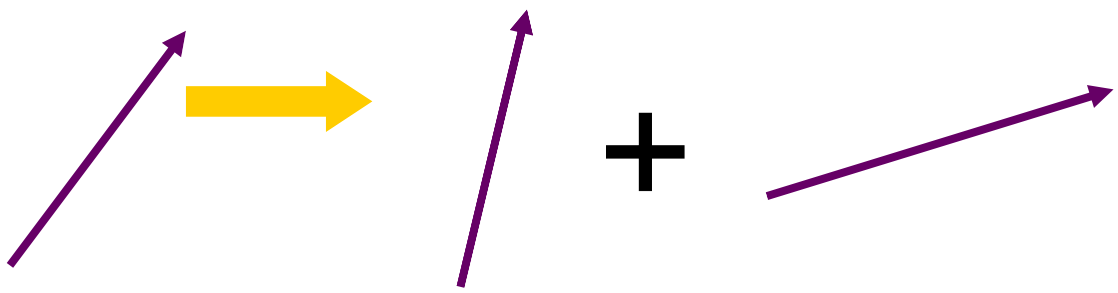
$$n_\uparrow n_\downarrow \Rightarrow n_\uparrow \times n_\downarrow$$

ML

Stratonovich-Hubbard transformation

Stratonovich-Hubbard transformation

$$\left|\Phi'\right\rangle = \exp[-\Delta_\beta H_1]\left|\Phi\right\rangle = \sum_s \left|\Phi(s)\right\rangle$$



branching occurs

Basis Generation in Slater Determinant Representation

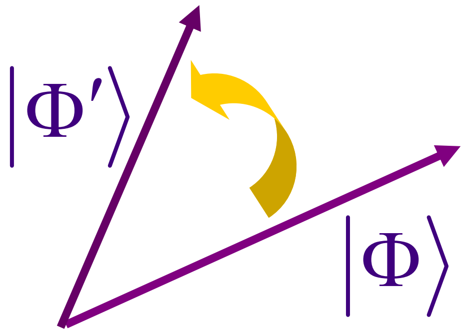
$$\left|\Phi\right\rangle = \lim_{p\to\infty}[\exp[-\tau H]]^{p}\left|\Phi_0\right\rangle$$

$$\exp[-\tau H] \approx \exp[-\tau H_K]\exp[-\tau H_U]$$

In Slater determinant representation

Kinetic energy

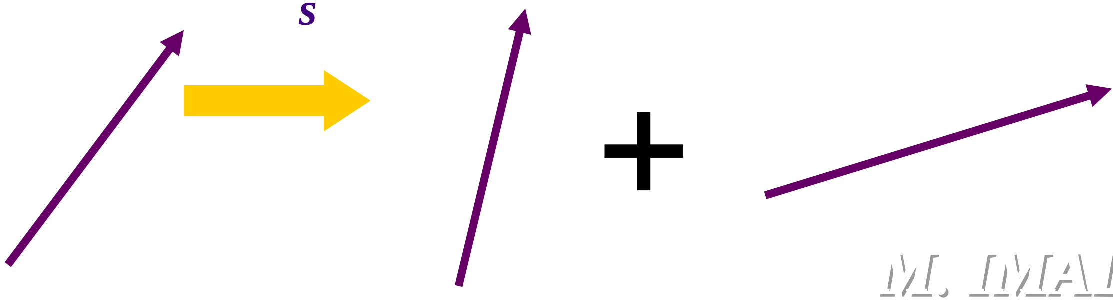
$$\left|\Phi'\right\rangle = \exp[-\tau H_K]\left|\Phi\right\rangle$$



Interaction energy

Stratonovich-Hubbard transformation

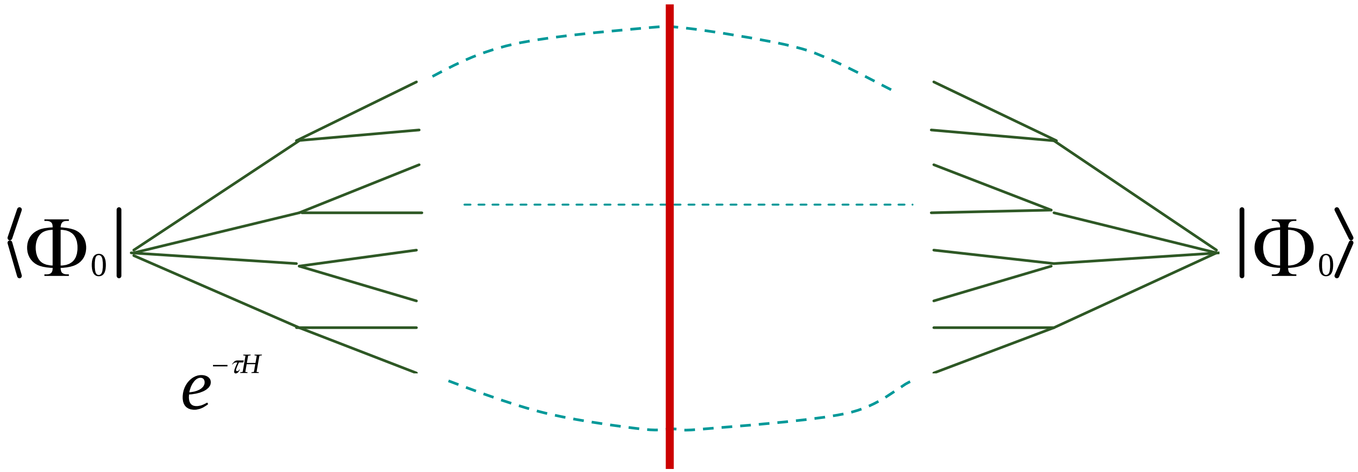
$$\left|\Phi'\right\rangle = \exp[-\tau H_U]\left|\Phi\right\rangle = \sum_s \left|\Phi(s)\right\rangle \text{ ; branching}$$



Ground State Algorithm by Auxiliary Fields of Path Integral

ground state

$$\left|\Phi\right\rangle = \lim_{p\to\infty}[\exp[-\Delta_\beta H]]^p \left|\Phi_0\right\rangle$$



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Matrix Elements in Canonical Ensemble

Trace out Fermion degrees of freedom
leaving auxiliary fields

$$b_0 = \exp[-\Delta_\beta H_K]$$

$$b_1 = \exp[-\Delta_\beta H_U(\{s\})]$$

density matrix

$$\rho(\beta;\varphi) = \sum_{\{s\}} W_\uparrow W_\downarrow,$$

$$W_\sigma = \det({}^t\Phi_\sigma B_{\sigma 1} B_{\sigma 2} \cdots B_{\sigma p} \Phi_\sigma)$$

$$B_{\sigma l} = b_0 b_{1\sigma}(s_1(l), s_2(l), \cdots, s_N(l)) b_0$$

Path integral in grand canonical ensemble

valid at finite temperature

$$\beta = p\Delta_\beta$$

$$\mathrm{Tr}\rho(\beta;\varphi) = \sum_{\{s\}} W_\uparrow W_\downarrow,$$

$$W_\sigma = \det(I + B_{\sigma 1} B_{\sigma 2} \cdots B_{\sigma p})$$

$$B_{\sigma l} = b_0 b_{1\sigma}(s_1(l), s_2(l), \cdots, s_N(l)) b_0$$

$$e^{-\Delta_\beta H_l(\tau_l)} = B_l$$

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Full summation over path integral

$$B = e^{\Delta_\beta H_K/2} e^{-\Delta_\beta H_U^{(\{s\})}} e^{-\Delta_\beta H_K/2}$$

$$\rho = \sum_{\{s\}} \prod_{l=1}^{p} B(\tau_l)$$

summation over all $\{s\}$

Numerical Algorithms

Summation over all
the Stratonovich-Auxiliary variable

requires 2^{Np} terms summations

Monte Carlo sampling ➡ **quantum Monte Carlo**

Renormalization (projection and truncation) of generated basis ➡ **path-integral renormalization group**

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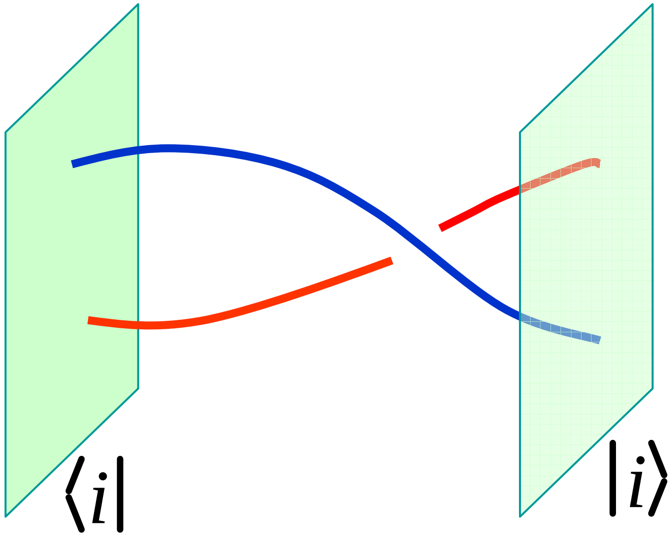
negative sign problem ← **Anticommuting Fermions**



$$W(A) = \langle i | e^{-\tau H} | j \rangle \langle j | e^{-\tau H} | k \rangle$$
$$\langle k | e^{-\tau H} \ldots A \ldots | i \rangle$$

$$W(1) < 0$$

Average sign decreases exponentially with increasing N, β

$$\langle A \rangle = \frac{\sum_s W_s(A)}{\sum_s W_s(1)} \approx \frac{0}{0}$$

Large statistical error

Difficulty in QMC

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Path-Integral Renormalization Group (PIRG)

Kashima et al. JPSJ 69 (2000)2723; 70(2001)2287

Numerical Framework of PIRG

Kashima et al. JPSJ 69 (2000)2723; 70(2001)2287

$$\left|\Phi\right\rangle = \sum_i^L c_i \left|\varphi_i\right\rangle$$

Optimize $\left|\Phi\right\rangle$ at fixed L

Increase L

Extrapolation

$$E = \frac{\left\langle\Phi\right|H\left|\Phi\right\rangle}{\left\langle\Phi\middle|\Phi\right\rangle} \qquad \left\langle A\right\rangle = \frac{\left\langle\Phi\right|A\left|\Phi\right\rangle}{\left\langle\Phi\middle|\Phi\right\rangle}$$

variational

$$\left\langle\varphi_i\right|A\left|\varphi_j\right\rangle, \left\langle\varphi_i\middle|\varphi_j\right\rangle$$

Easily computable

ex. Slater determinant

No negative-sign problem

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Basis Generation in Slater Determinant Representation

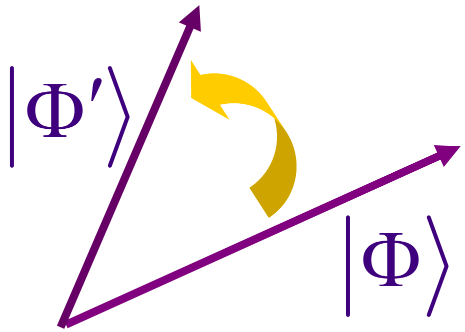
$$|\Phi\rangle = \lim_{p\to\infty}[\exp[-\tau H]]^p |\Phi_0\rangle$$ path integral

$$\exp[-\tau H] \approx \exp[-\tau H_t]\exp[-\tau H_U]$$

In Slater determinant representation

Kinetic energy

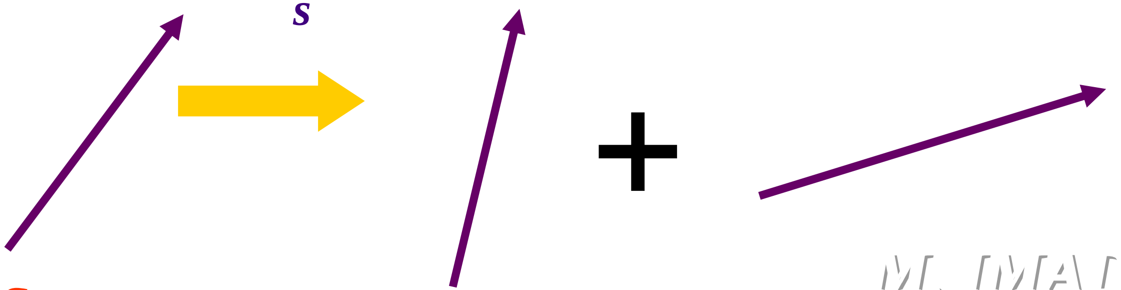
$$|\Phi'\rangle = \exp[-\tau H_t]|\Phi\rangle$$



Interaction energy

Stratonovich-Hubbard transformation

$$|\Phi'\rangle = \exp[-\tau H_U]|\Phi\rangle = \sum_s |\Phi(s)\rangle$$; branching



nonorthogonal basis

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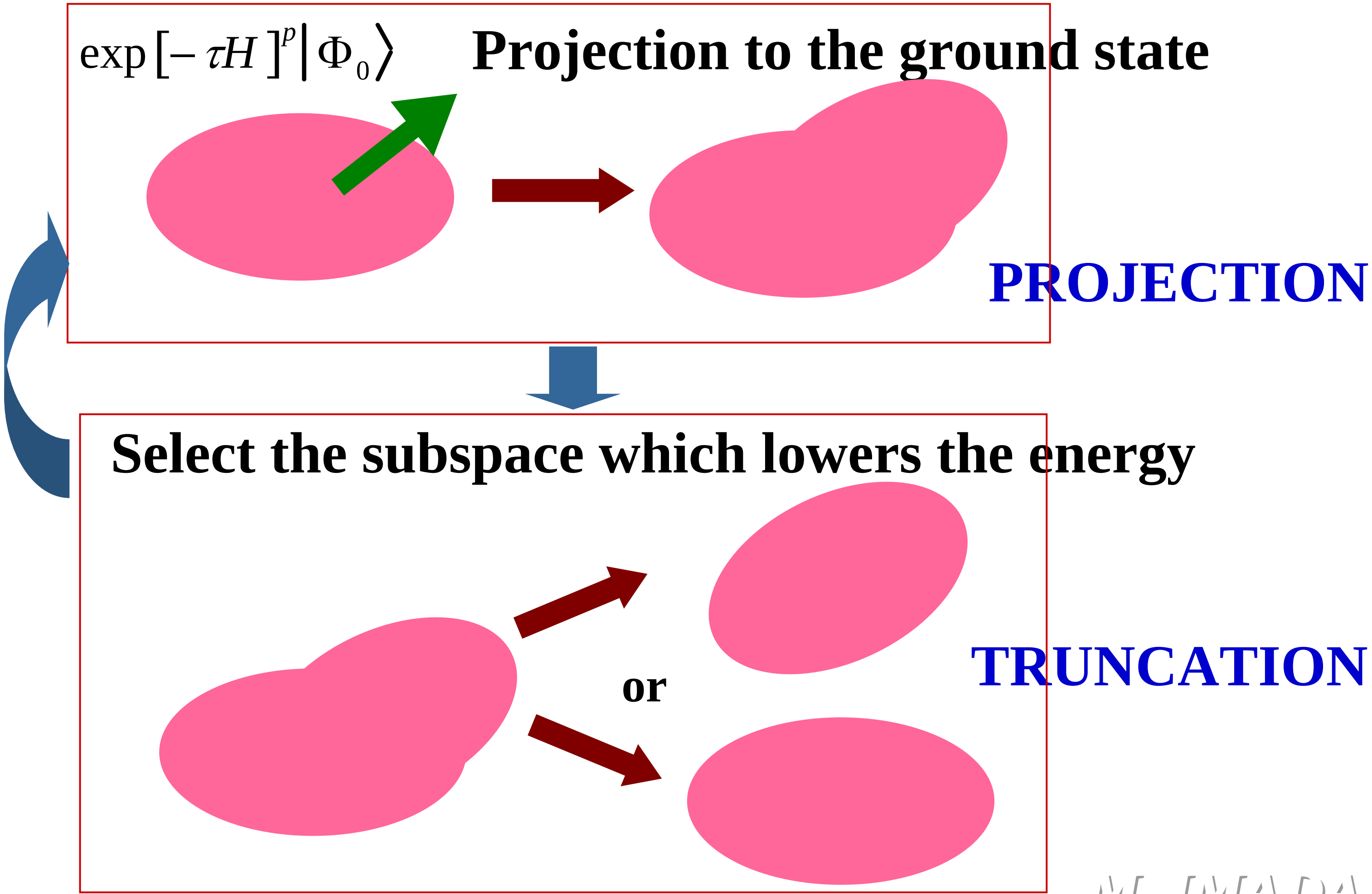
WF Renormalization
in the direction to imaginary time

$$|\Phi\rangle = \lim_{p\to\infty}[\exp[-\tau H]]^p |\Phi_0\rangle$$



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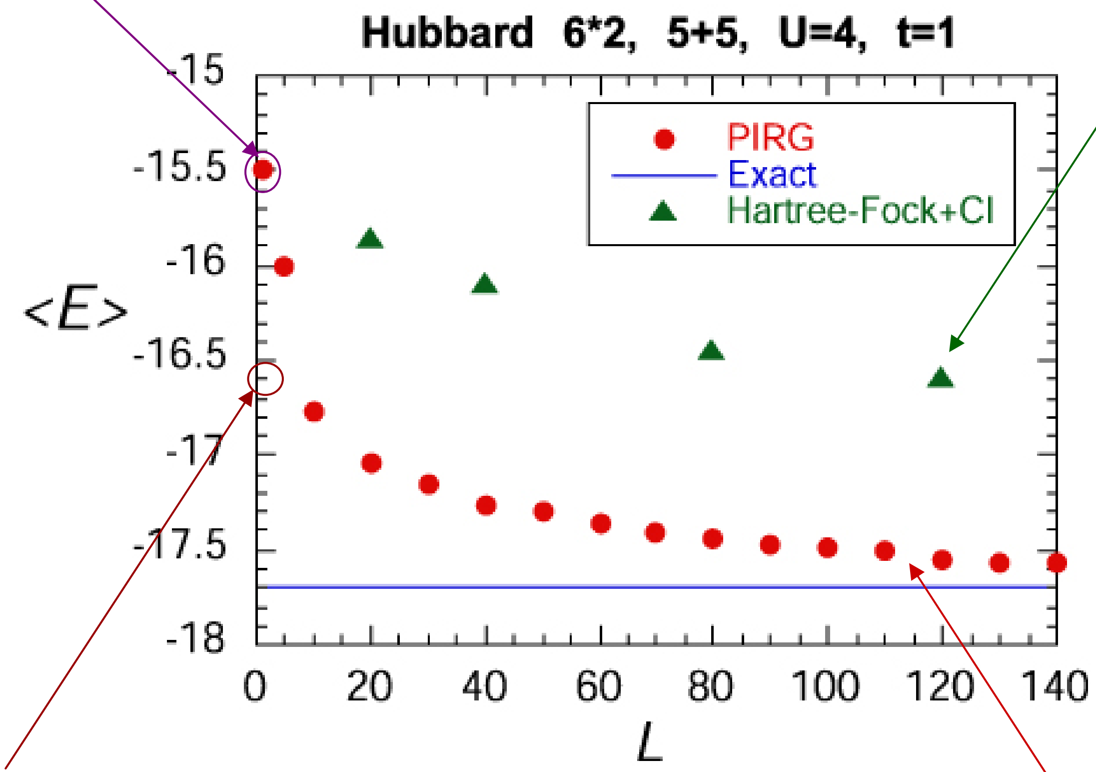
Comparison with Orthogonal Basis

Hartree-Fock energy

Orthogonal basis
= Configuration Interaction



with
Gutzwiller factor
(VMC)

Optimized non-orthogonal basis

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Renormalization procedure

At a fixed dimension, *L* in restricted Hilbert space in some representation, find the " fixed point " :

$$\left\langle \varphi_i \middle| \varphi_j \right\rangle \text{ and } \left\langle \varphi_i \middle| H \middle| \varphi_j \right\rangle$$ **"effective Hamiltonian"**

projection & truncation → $$\left|\Phi\right\rangle = \sum_i^L c_i \left|\varphi_i\right\rangle$$ **ground state of "effective Hamiltonian"**

w.f. renormalization, hamiltonian matrix renormalization

Renormalization in energy; filtering out high energy mode

c.f. in usual RG, one finds a fixed point rep. in the scaled but essentially fixed rep.

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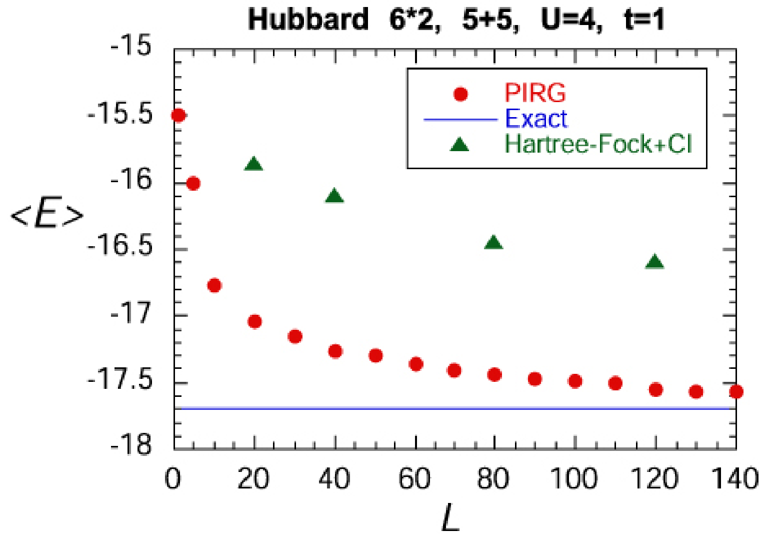
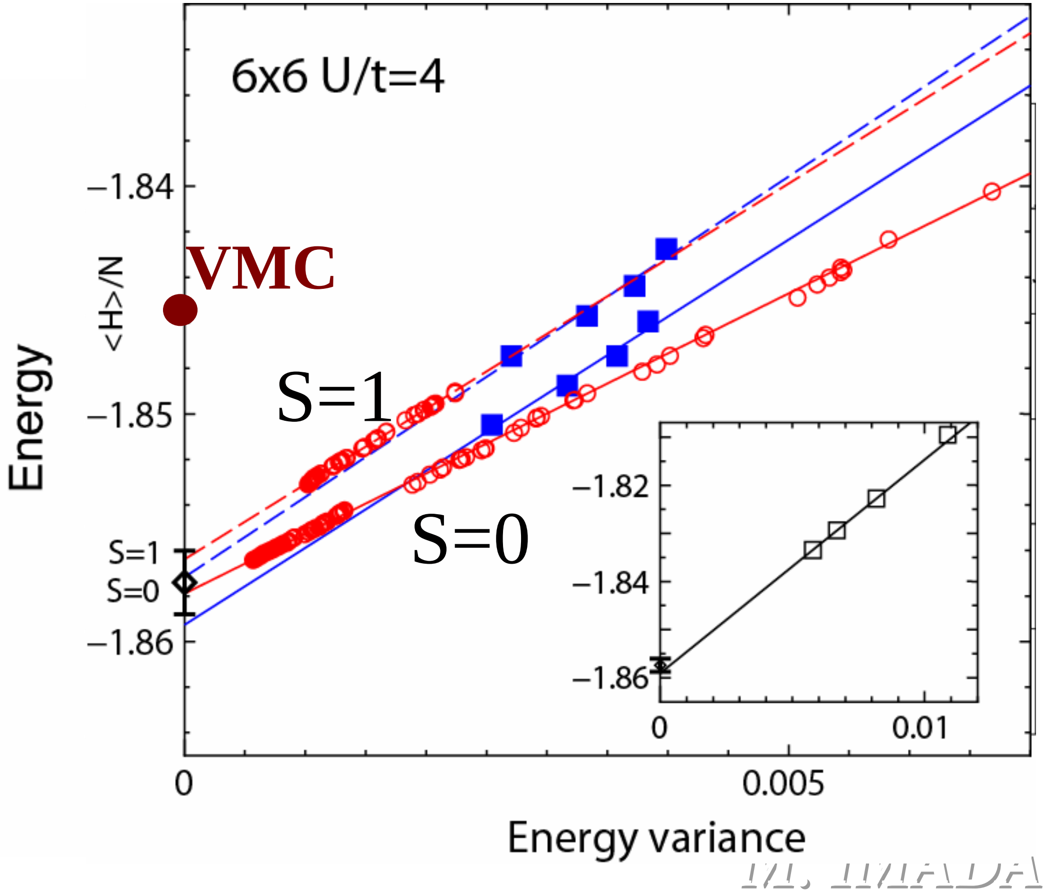
Extrapolation to $L \to \infty$

$\Delta_E = \left(\langle E^2 \rangle - \langle E \rangle^2 \right) / \langle E \rangle^2$: **Extrapolation with energy variance**

$\langle E \rangle - E_0 \propto \Delta_E$: ***L* large**





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Quantum number projection

variational ground states in the restricted Hilbert space
do not necessarily preserve the original symmetries of *H*

How to restore the symmetries ?

Quantum number projection operator

$$\mathcal{L}\left|\psi\right\rangle,$$

$$\left\langle\psi\right|\mathcal{L}\left|\psi\right\rangle, \ \left\langle\psi\right|\hat{H}\mathcal{L}\left|\psi\right\rangle, \ \left\langle\psi\right|\hat{O}\mathcal{L}\left|\psi\right\rangle,$$

$$\mathcal{L}^2 = \mathcal{L}$$

Mizusaki and Imada
PRB69, 125110 (2004)

Momentum Projection

$$\mathcal{L}^{\vec{k}} = \frac{1}{\mathcal{N}} \sum_j e^{i(\vec{K}-\vec{k})\vec{R}_j}$$

K; momentum operator

$$\frac{1}{\mathcal{N}} \sum_j e^{i\vec{K}\vec{R}_j} |\phi(0)\rangle = |\phi(j)\rangle$$

j spatial translation

$$\left\{ \begin{array}{c} N \\ H \\ O \end{array} \right\} = \frac{1}{\mathcal{N}} \sum_j e^{-i\vec{k}\vec{R}_j} \langle\phi| \left\{ \begin{array}{c} 1 \\ \hat{H} \\ \hat{O} \end{array} \right\} |\phi(j)\rangle$$

Spin rotation

Wigner's *D* function

$$L^S_{MK} \equiv \frac{2S+1}{8\pi^2}\int d\Omega D^{S*}_{MK}(\Omega)R(\Omega)$$

$\Omega = (\alpha, \beta, \gamma)$ **Euler angle**

$$R(\Omega) = e^{i\alpha S_z}e^{i\beta S_y}e^{i\gamma S_z}$$

$$D^S_{MK}(\Omega) = \langle SM|R(\Omega)|SK\rangle = e^{i\alpha M}e^{i\gamma K}d^S_{MK}(\beta)$$

$$d^S_{MK}(\beta) = \left\langle SM\left|e^{i\beta S_y}\right|SK\right\rangle.$$

$$L^S_{N_0 M}L^S_{M' N_0} = L^S_{N_0, N_0}\delta_{MM'} \qquad N_0 = S_z$$

Spin projection

$$\mathcal{L}^S_{N_0 N_0} \equiv \frac{2S+1}{2}\int_0^\pi d\beta \sin\beta d^S_{N_0 N_0}(\beta) e^{i\beta S_y}.$$

$$\left\{ \begin{array}{c} N \\ H \\ O \end{array} \right\} = \frac{2S+1}{2}\int_0^\pi d\beta \sin\beta d^S_{N_0 N_0}(\beta) \langle\phi'| \left\{ \begin{array}{c} 1 \\ \hat{H} \\ \hat{O} \end{array} \right\} |\phi(\beta)\rangle$$

$$|\phi(\beta)\rangle = e^{i\beta S_y}|\phi\rangle.$$

$$d^S_{0,0}(\beta) = P_S(\cos\beta)$$

Legendre polynomial

Quantum-Number Projected PIRG (QP-PIRG)

Mizusaki and Imada
PRB69, 125110 (2004)

$$|\psi_g\rangle = \lim_{\tau\to\infty} e^{-\tau H}|\phi_{initial}\rangle$$

$$\lim_{\tau\to\infty} e^{-\tau H}\mathcal{L}\,|\phi_{initial}\rangle$$

is replaced with

$$\lim_{\tau\to\infty}[\mathcal{L}e^{-\Delta\tau H_K}\prod_i \mathcal{L}e^{-\Delta\tau H_{Ui}}]^M\,|\phi_{initial}\rangle$$

Yrast state;
lowest energy state with specified quantum number

Quantum Number Projection + PIRG

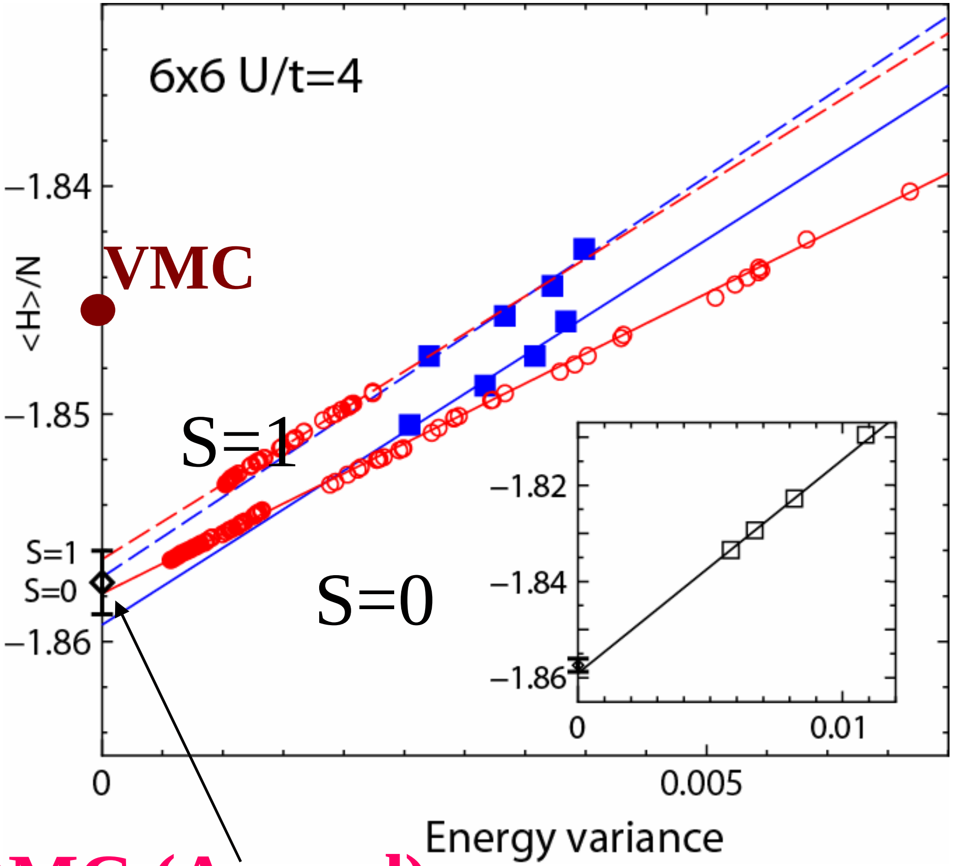
Spin, Momentum, …

QMC -1.8574(14)

QP-PIRG -1.85790 (2)

PIRG+QP

QP-PIRG



QMC (Assaad)

Excited States

Energy Dispersion

Yrast states

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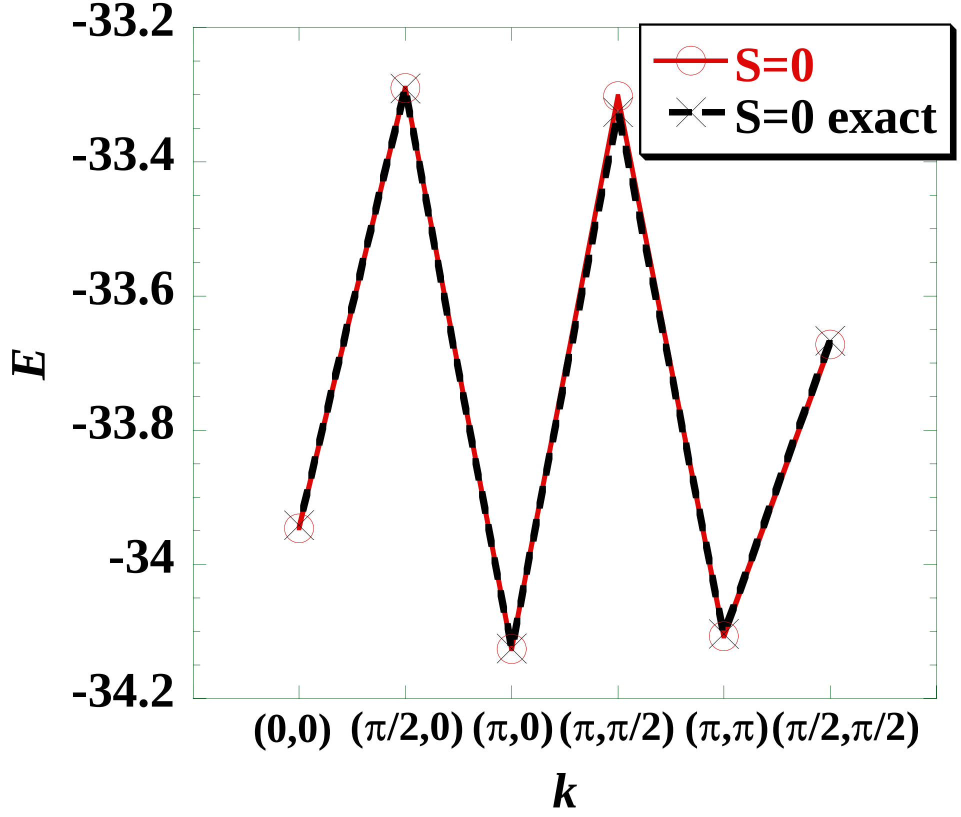
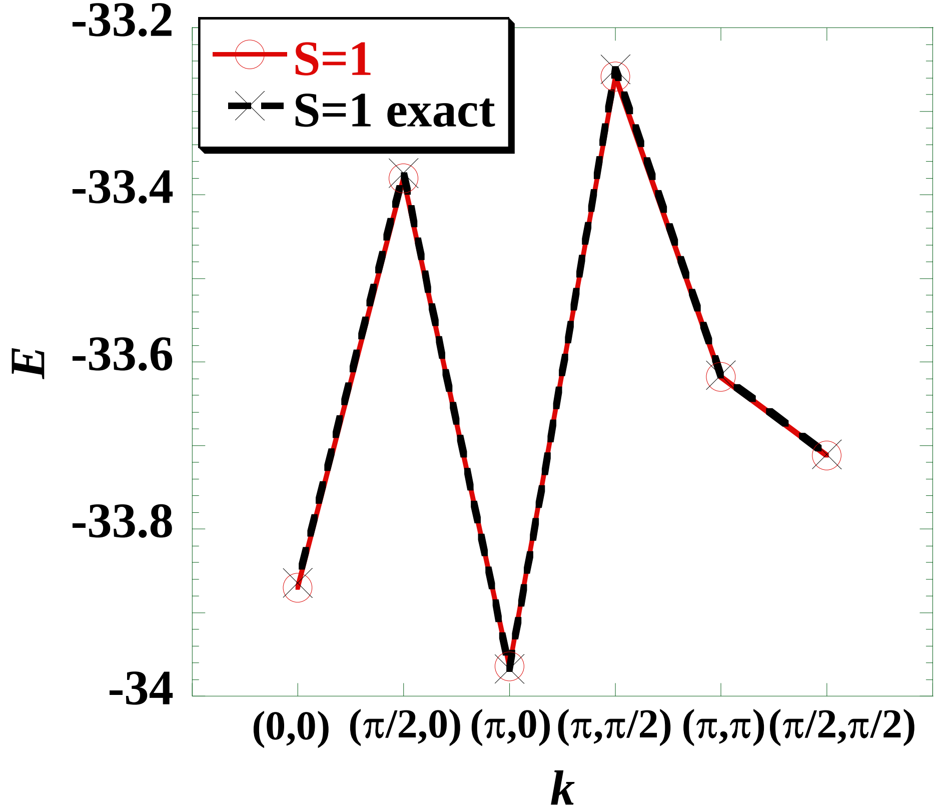
Excitation Spectra, Dispersion





4×4 Hubbard

U=5.7, t=1, t'=0.5

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Grand Canonical Ensemble

Watanabe, MI;
JPSJ 73 (2004) 1251

$$\mathcal{H} = H - \mu \hat{N}_e$$

Particle-hole transformation $\begin{cases} c_{k\uparrow} \rightarrow c_k \\ c_{-k\downarrow} \rightarrow d_k^+ \end{cases}$

Transformed Hamiltonian:

$$\mathcal{H} = H_t + H_U - \left(\frac{U}{4} + \mu\right) N$$

$$H_t = -\sum_{\langle ij \rangle} t_{ij} \left(c_i^+ c_j + c_j^+ c_i\right) + \left(\frac{U}{2} - \mu\right) \sum_i c_i^+ c_i$$
$$+ \sum_{\langle ij \rangle} t_{ij} \left(d_i^+ d_j + d_j^+ d_i\right) + \left(\frac{U}{2} + \mu\right) \sum_i d_i^+ d_i$$

$$H_U = -U \sum_i c_i^+ c_i d_i^+ d_i$$

Extended basis

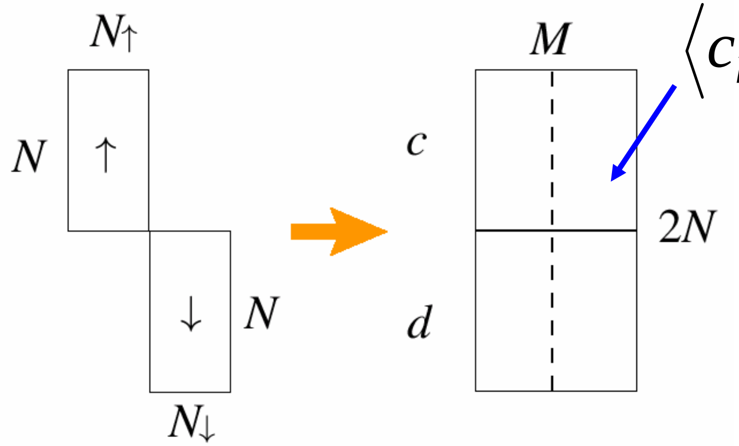
$$\left|\phi\right\rangle = \prod_{k=1}^{M}\left(\sum_{i=1}^{2N}[\phi]_{ik}\tilde{c}_i^{+}\right)\left|0\right\rangle$$

$$\tilde{c}_i^{+} = \begin{cases} c_i^{+} & \text{for } i = 1,\ldots,N \\ d_{i-N}^{+} & \text{for } i = N+1,\ldots,2N \end{cases}$$

canonical

grand canonical

$[\phi]_{ik}$:



$$\left\langle c_k^{+} d_k \right\rangle = \left\langle c_{k\uparrow}^{+} c_{-k\downarrow}^{+} \right\rangle$$

cf. superconductivity

Yokoyama & Shiba(1988)

Total electron number

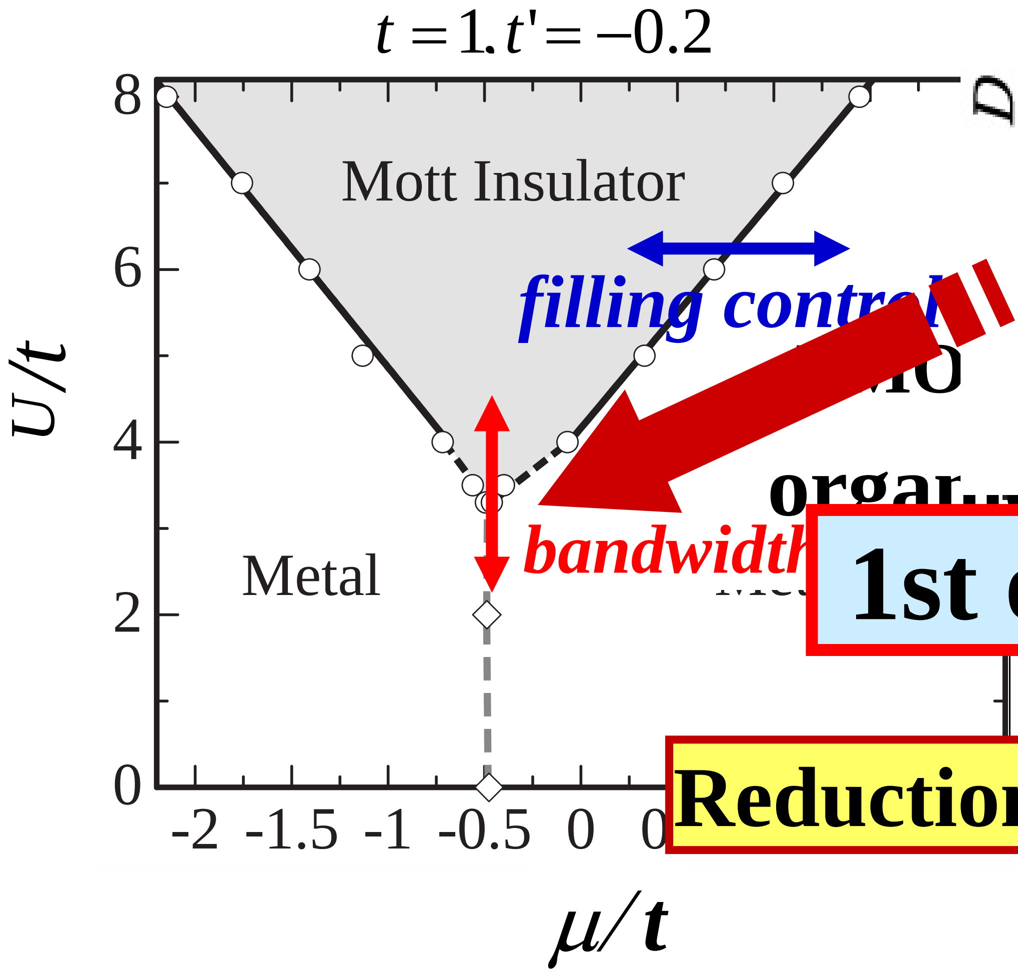
$$N_e = \sum_{i\sigma}\left\langle c_{i\sigma}^{+} c_{i\sigma}\right\rangle = N + \sum_{i}\left\langle c_i^{+} c_i - d_i^{+} d_i\right\rangle$$

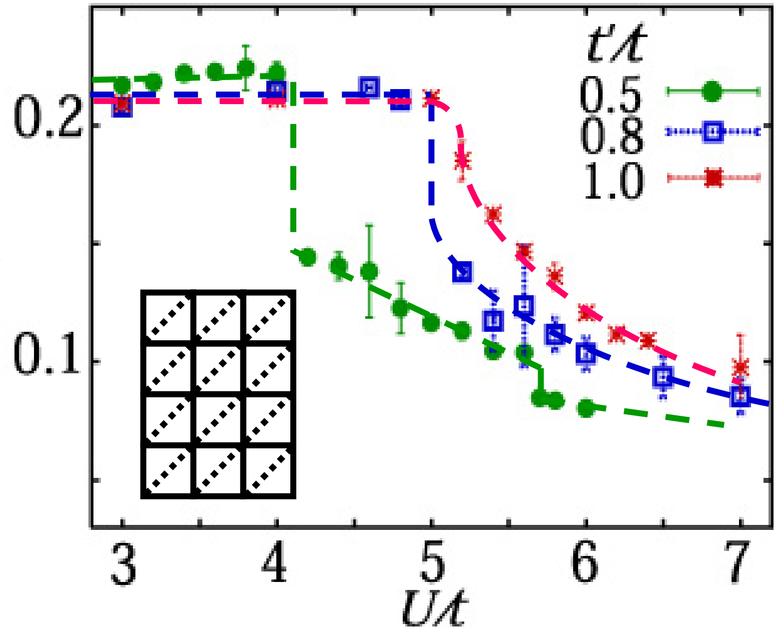
Several Applications

Hubbard Model

Phase Diagram of Mott Transition in the 2D Hubbard model; *T*=0

PIRG numerical results





1st order transition

V shape boundary

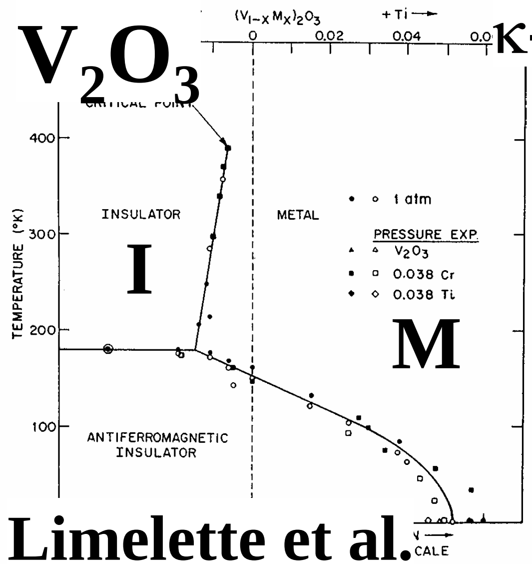
Reduction of jump for larger *t'*

Watanabe, MI

JPSJ**73**(2004)1251

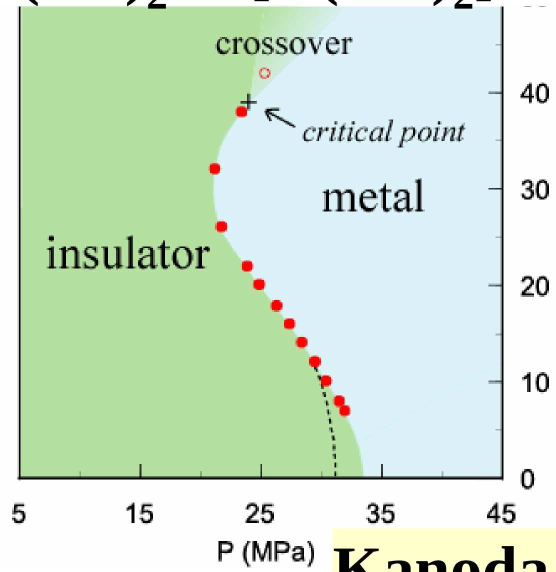
Mott transition in experiments

V_2O_3



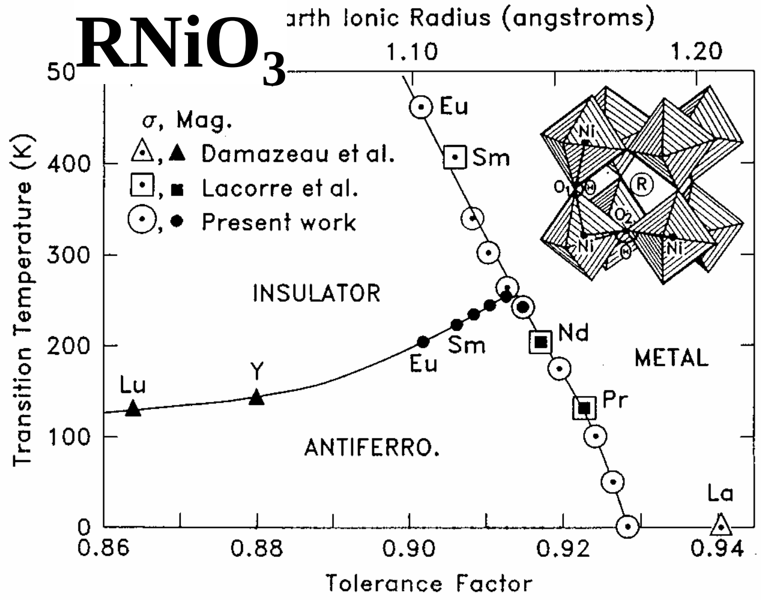
Limelette et al.

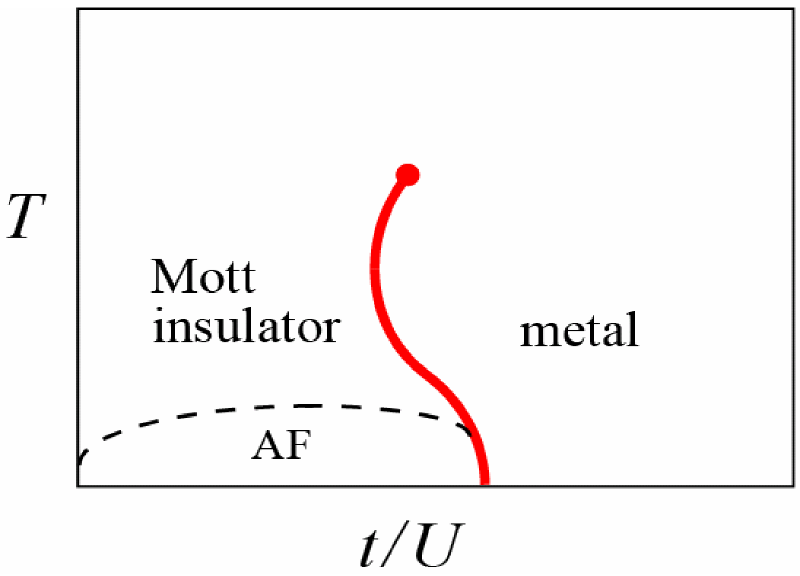
κ-$(ET)_2Cu[N(CN)_2]Cl$



Kanoda et al.

$RNiO_3$





Reduction of *Tc*
for larger frustration

pyrochlore; continuous

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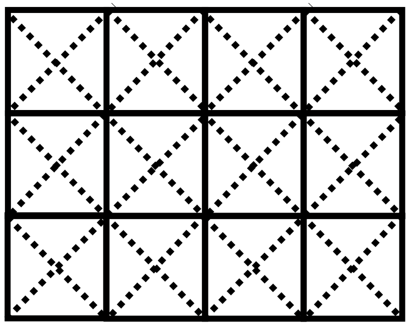
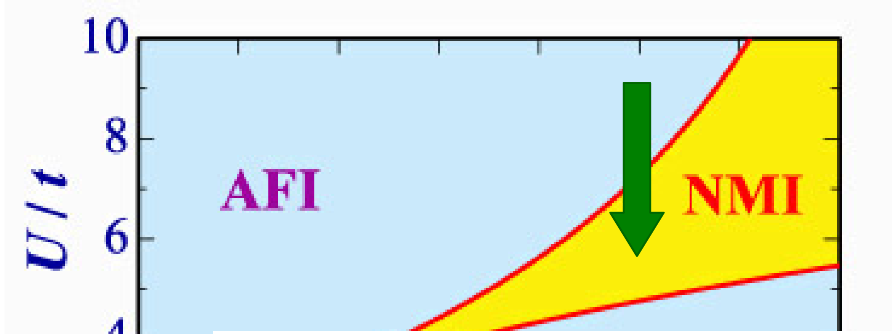
Phase Diagram of Frustrated Hubbard Model at ½ Filling



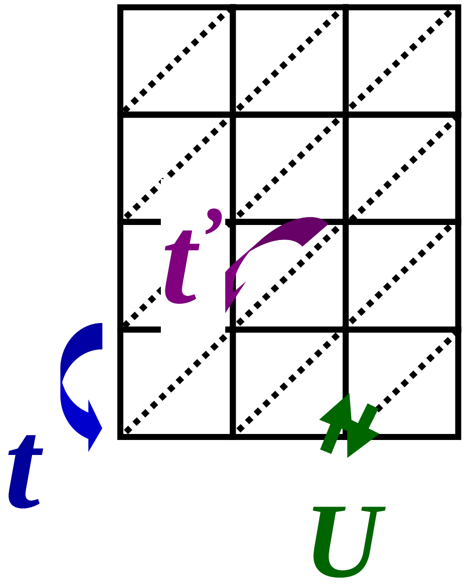
Frustrated square lattice

Kashima et al.

JPSJ 70 (2001) 3052



Spin melting
before charge melting



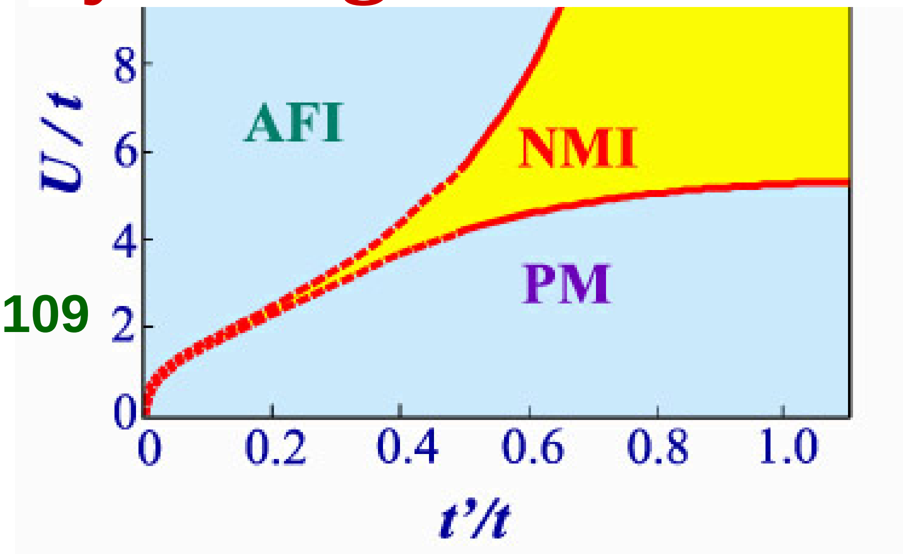
Anisotropic triangular lattice

Morita et al.

JPSJ 71(2002) 2109

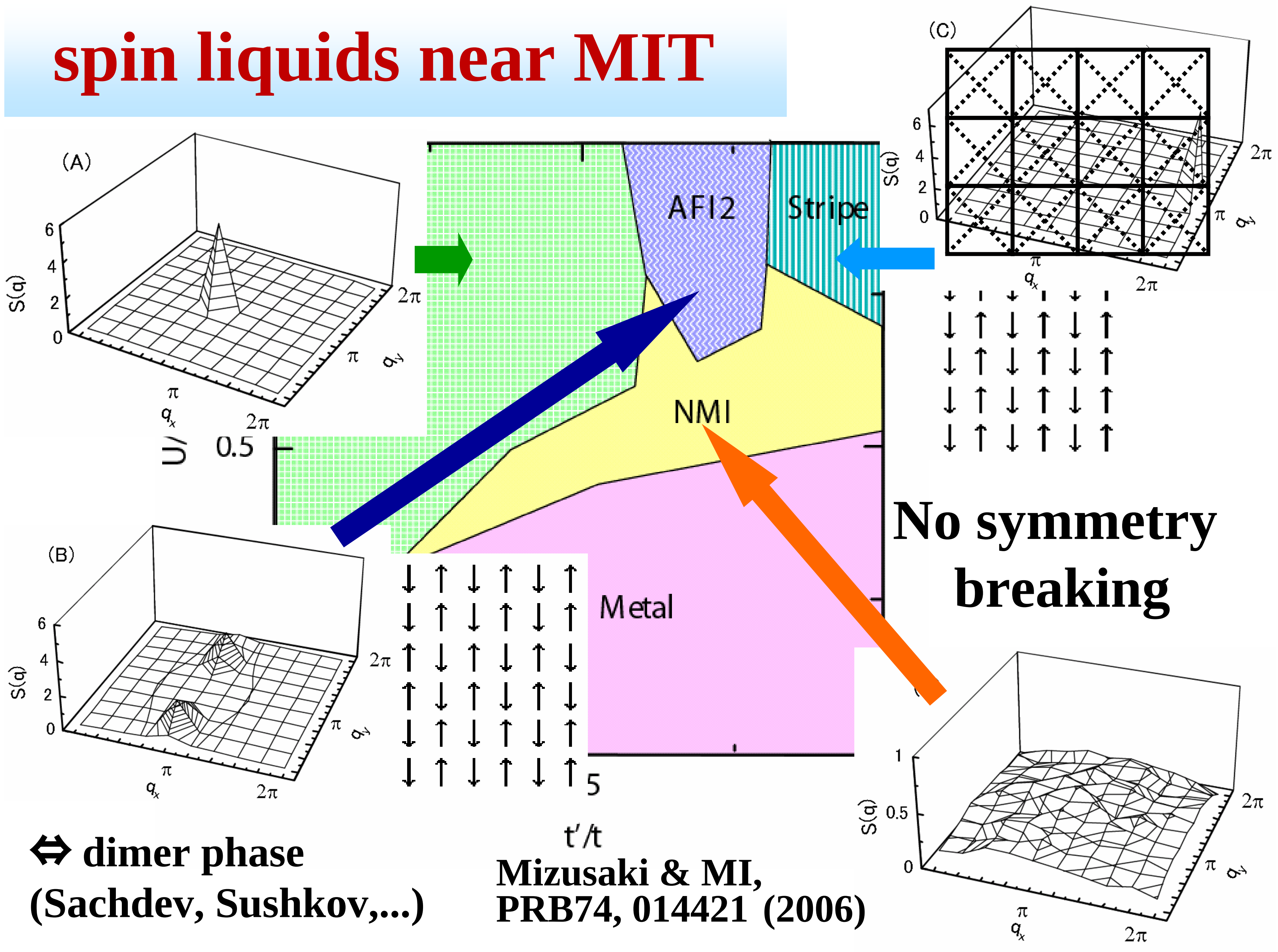
HF;V

Quantum melting by charge fluctuations



Nonmagnetic Mott insulator phase

spin liquids near MIT

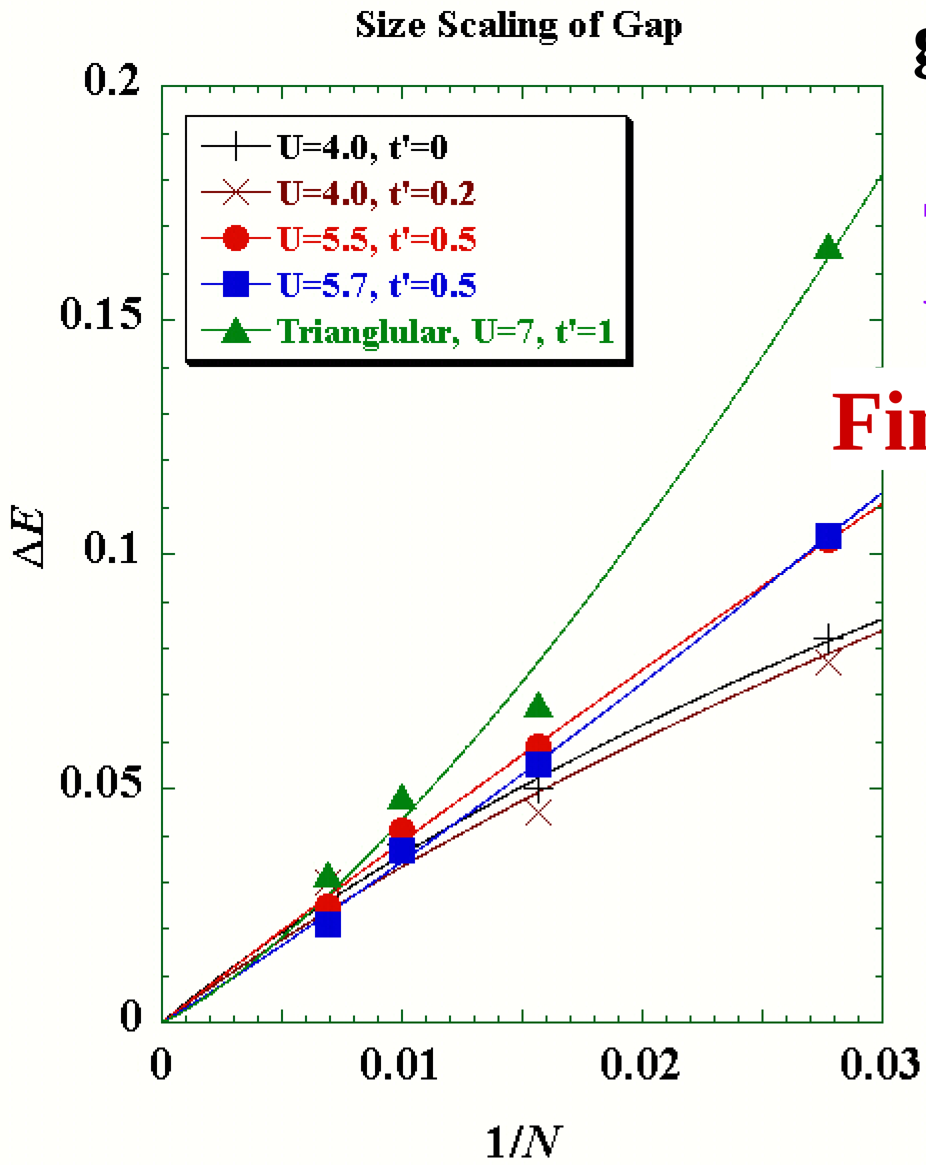


No symmetry breaking

⇔ dimer phase
(Sachdev, Sushkov,...)

Mizusaki & MI,
PRB74, 014421 (2006)

Nature of spin liquid phase: Spin-gapless phase



gapless spin excitations

$\Delta E \sim 1/N$

Triplet excitation gap collapses with increasing system size

Finite uniform susceptibility

Mizusaki & MI, PRB74, 014421 (2006)

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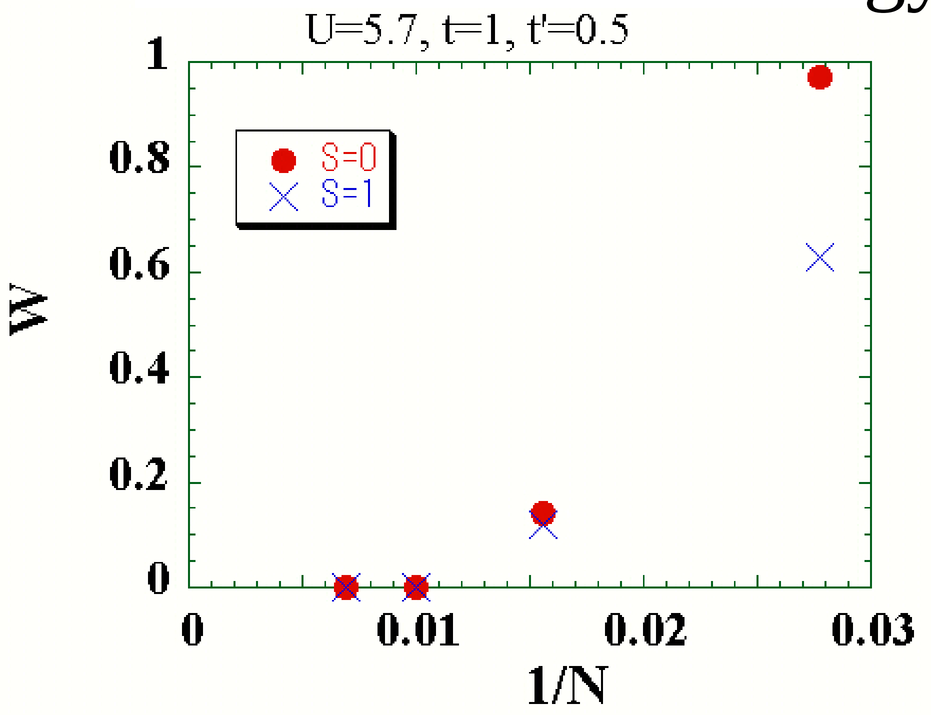
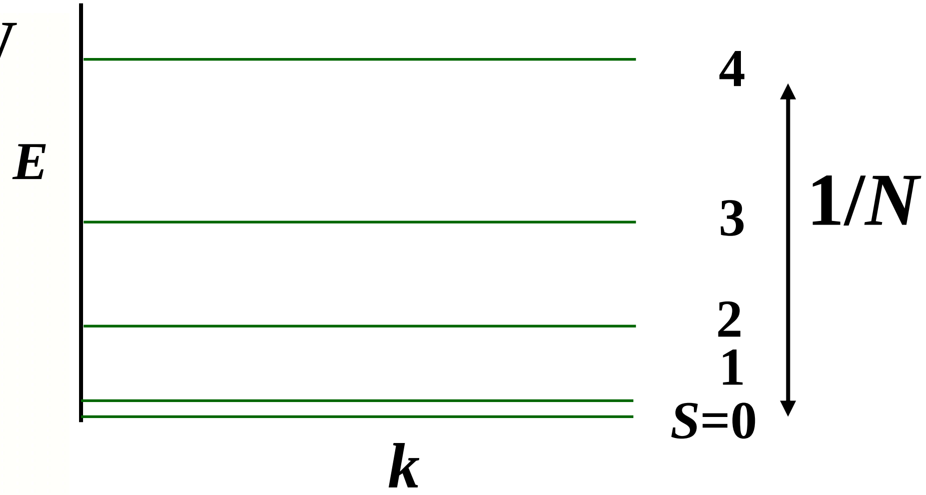
k-dependence of gapless excitation

width of excitation energy





Gapless excitations with double hierarchy structure

cf. kagome, pyrochlore;
Chalker et al., Canals, Lacrois
Harris et al., Tsunetsugu

Very small dispersion (incoherent excitation)?

or

continuum of excitation (spinon Stoner excitation)?

Coherence

gapless excitation structure

spin renormalization factor

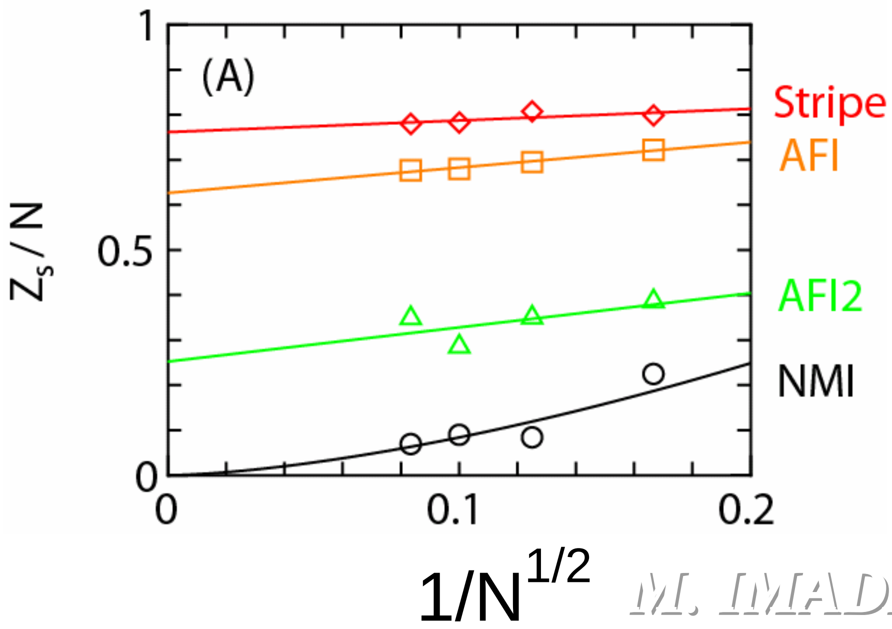
$$Z_s = |< S=1, q \,|\, \sum_k c^{\dagger}{}_{\uparrow}(k+q) c_{\uparrow}(k) - c^{\dagger}{}_{\downarrow}(k+q) c_{\downarrow}(k) \,|\, S=0, q=0 >|$$

$$= |< S=1, q \,|\, \sum_k S^{+}(q) \,|\, S=0, q=0 >|$$

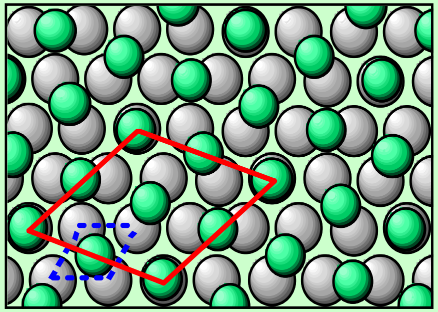
particle-hole excitation

no fractionalization

$Zs/\sqrt{N} \to 0$ for $N \to \infty$



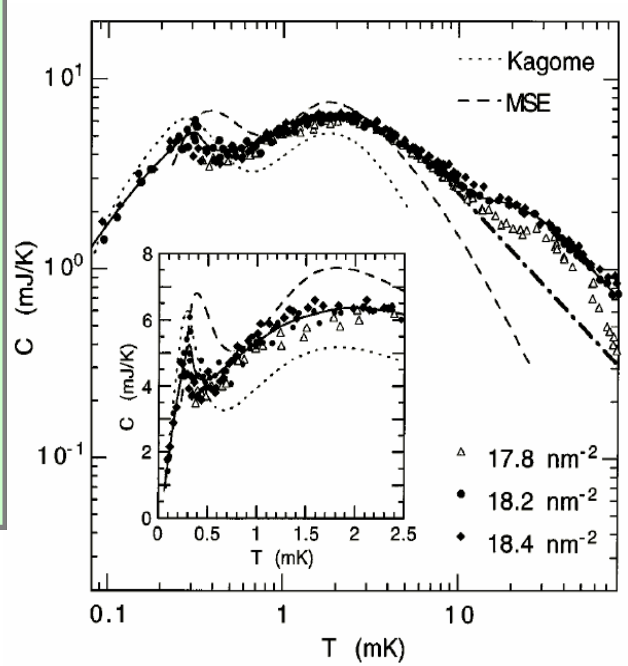
Exotic Spin Liquid at Registered Phase



C2: $\sqrt{7}\times\sqrt{7}$ commensurate phase

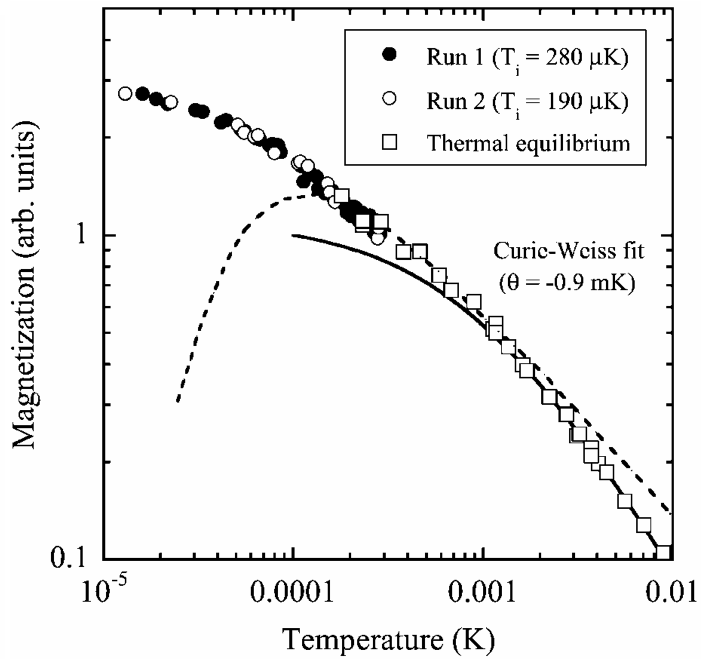
- 2nd layer atom
- 1st layer atom

specific heat



K. Ishida et al., PRL 79, 3451 (1997)

magnetic susceptibility



Masutomi, Karaki and Ishimoto PRL (2004)

T > 10μK; no order

gapless excitation

Exchange coupling ~ 10mK

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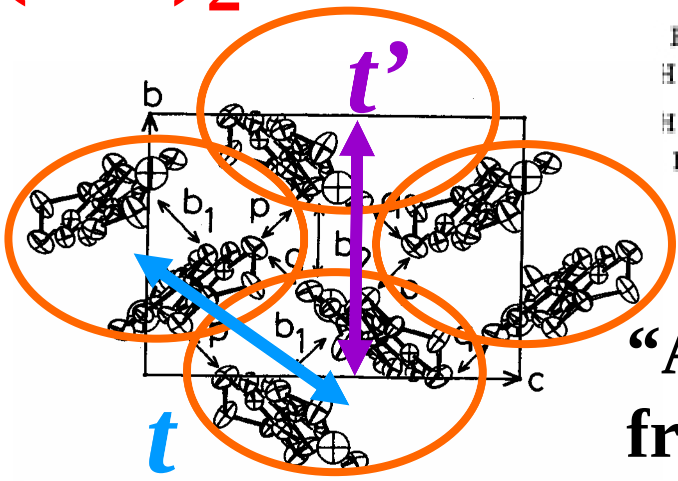
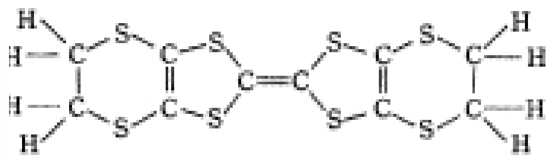
κ−$(ET)_2X$

X= $N(CN)_2Br$
= $N(CN)_2Cl$
= $Cu(NCS)_2$





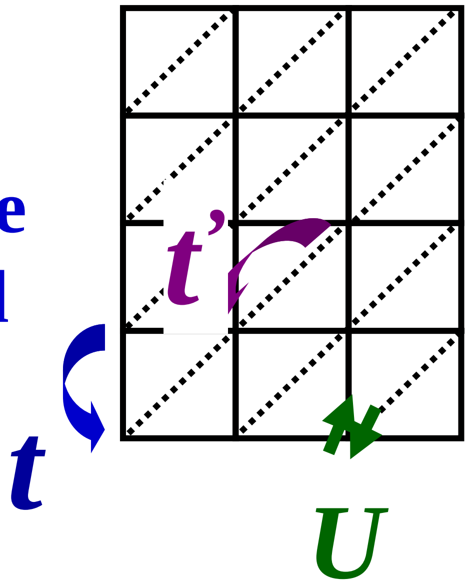
Dimerization

"Approximate" single band 2D system from antibonding orbital at a dimer molecule

Mori

Half filled

anisotropic triangular lattice with single band



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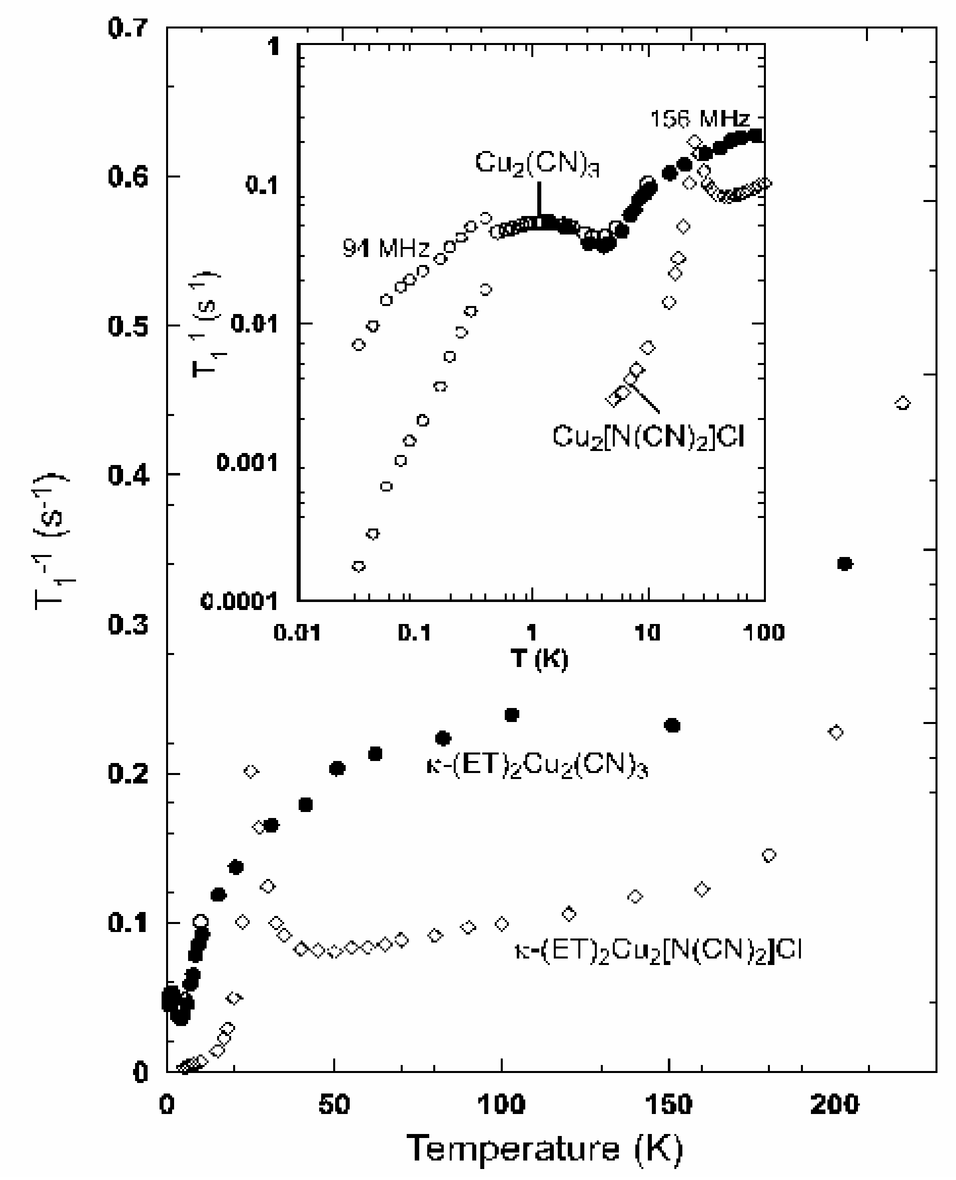
κ–$(ET)_2Cu_2(CN)_3$



X=$Cu_2(CN)_3$

$t'/t \sim 1.0$,

(largest among ET family)

$U/t \sim 8$

Shimizu, Maesato,
Saito, Miyanaga, Kanoda (2003)

No signature of magnetic transition down to 0.03K

No long-ranged order
Gapless excitations

M. IMADA

Electronic Structure Calculation of Realistic Systems

Downfolded Hamiltonian

Imai, Solovyev, MI
PRL, 95 (2005) 176405

$$H = \sum_{kn} \varepsilon_{kn} c^{\dagger}_{kn} c_{kn} + \frac{1}{2} \sum_{k,k',n,m,n',m'} c^{\dagger}_{kn} c_{kn'} U_{nn',mm'}(k,k') c^{\dagger}_{k'm} c_{k'm'}$$

→ **solver; PIRG**

----
xy=1, yz=2, zx=3
----
interaction
(1) intra-orbital Coulomb interaction:
U(1)=2.772451, U(2)=2.583078, U(3)=2.583069
(2) inter-orbital Coulomb interaction:
U'(1,2)=1.346084, U'(1,3)=1.346081,
U'(2,3)=1.279618
(3) exchange and pair hopping:
J(1,2)=0.654524, J(1,3)=0.654524, J(2,3)=0.639163

level
-0.8468 -0.9288

degeneracy of *yz,zx*

hopping
vector: 1.000000 0.000000 0.000000
-0.2184 0.0000 0.0000
0.0000 -0.0451 0.0000
0.0000 0.0000 -0.1940
vector: 1.000000 1.000000 0.000000
-0.0753 0.0000 0.0000
0.0000 0.0094 0.0029
0.0000 0.0029 0.0094
vector: 0.500000 0.500000 1.638780
0.0020 0.0056 0.0056
0.0056 -0.0157 -0.0089
0.0056 -0.0089 -0.0157
vector: 2.000000 0.000000 0.000000
-0.0035 0.0000 0.0000
0.0000 0.0004 0.0000
0.0000 0.0000 0.0175

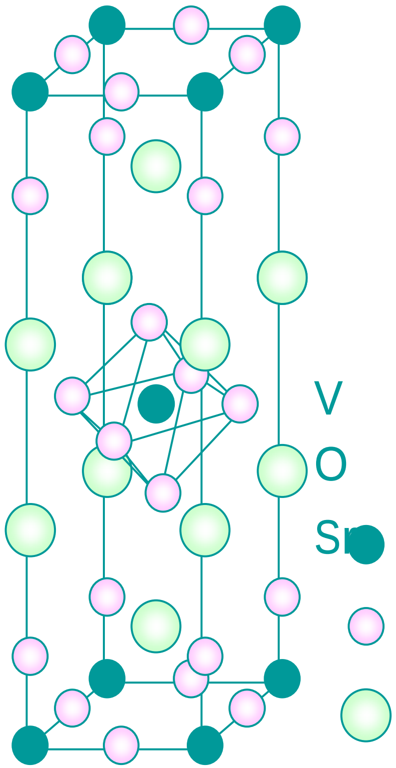
Renormalization factor

$$Z = [1 - \partial\Sigma/\partial\omega]^{-1} \approx 0.8$$

renormalization factors:
Z_{xy}=0.81 Z_{yz}=0.80

Sr_2VO_4

Similarity to high-T_c cuprates
Layered perovskite



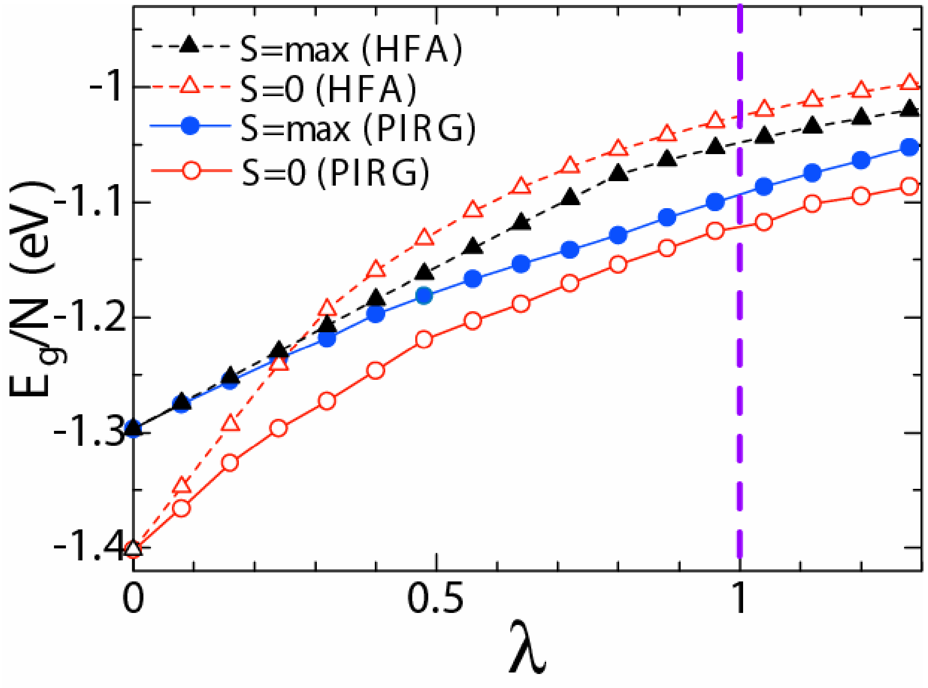
one 3*d* electron :
d ^{1} **system**

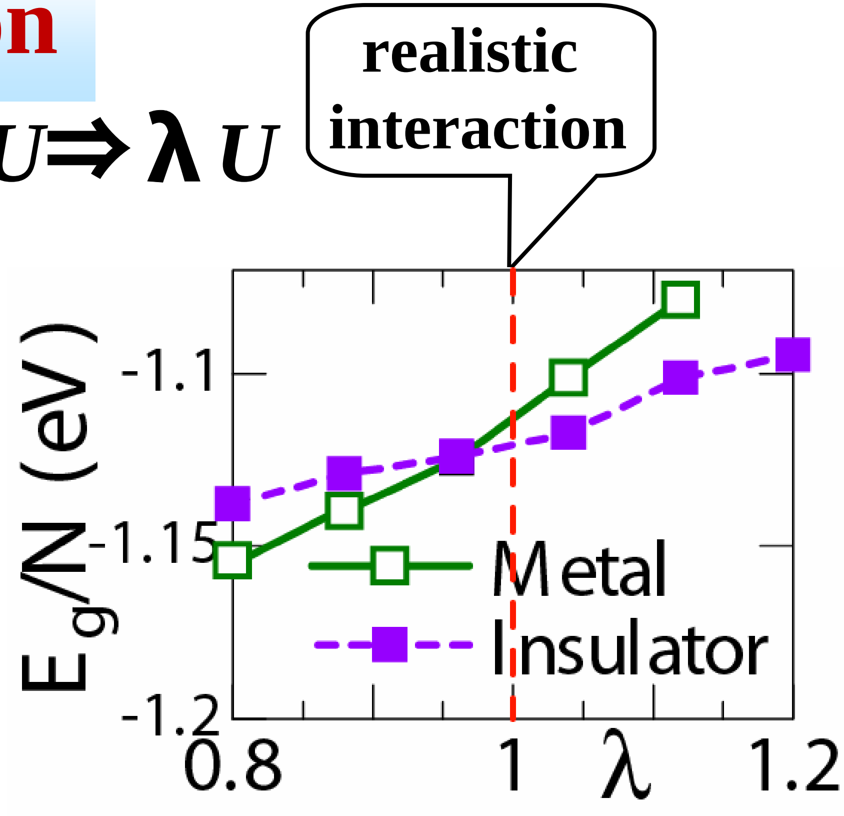
Nozaki et al. 1991

cuprates ; ***d*** ^{9} **system**
one 3*d* hole

Total energy comparison

λ:**interaction parameter** $U \Rightarrow \lambda U$





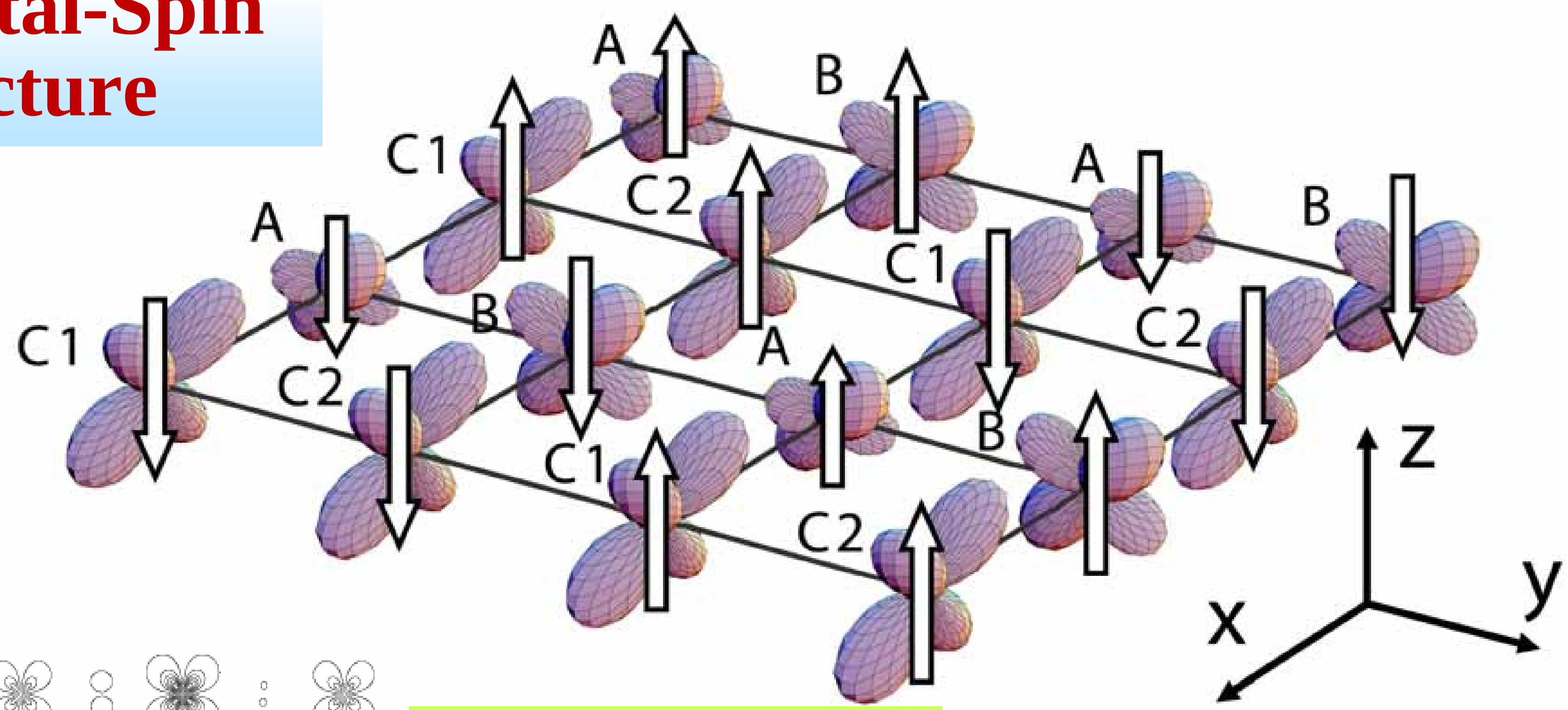
Spin singlet ground state

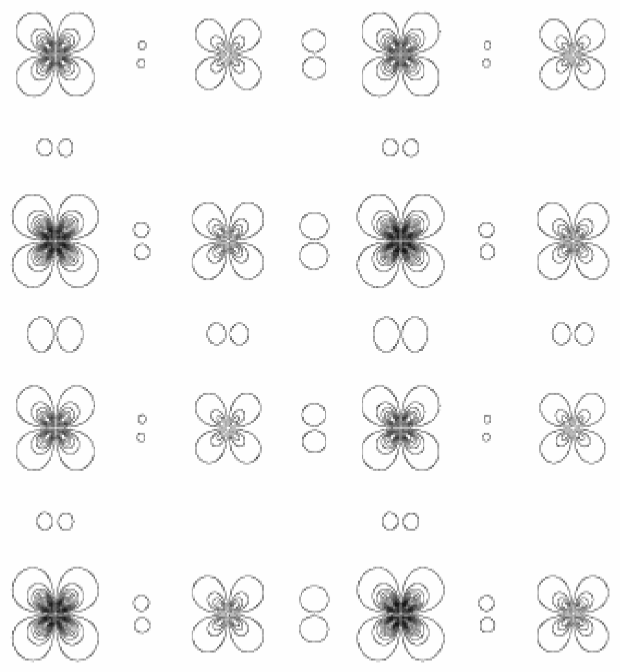
PIRG result; $\lambda_c \sim 0.9$

Close to the MI transition

Imai, Solovyev, MI
PRL, 95 (2005) 176405

Orbital-Spin Structure





orbital stripe & plaquette spin

charge density
on the mirror plane

4✕2 structure

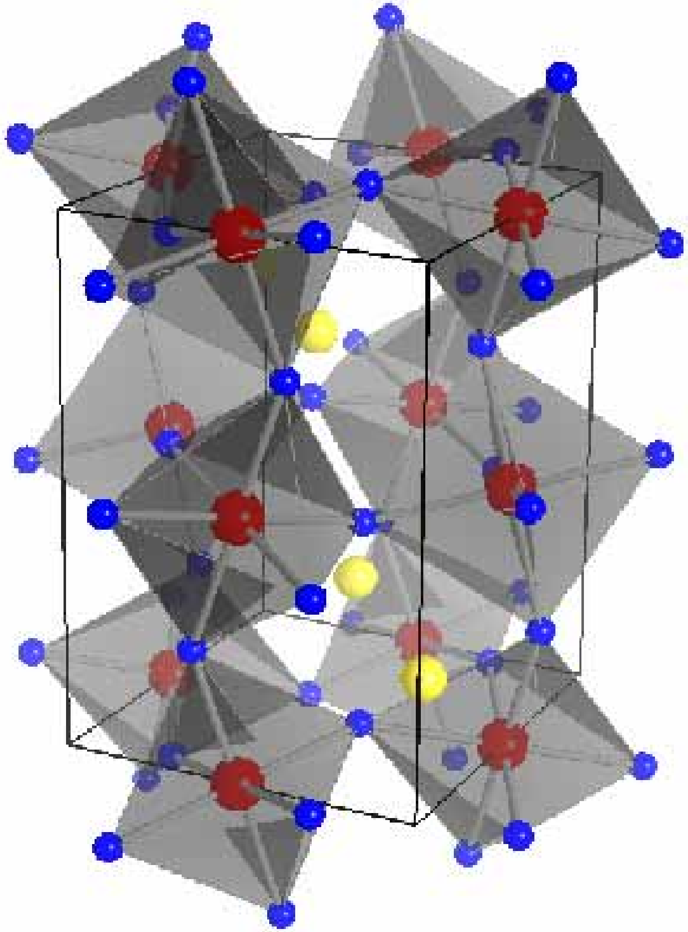
highly
nontrivial
structure

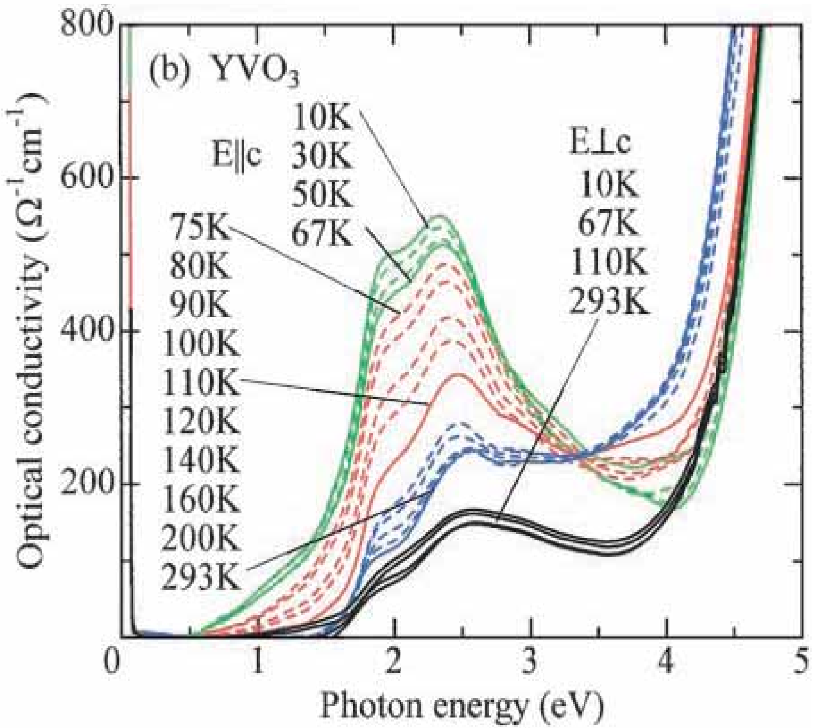
Electronic Structure by Our Method I

Sr_2VO_4	conduction	gap	magnetism
LDA	metal	0	para
Hartree-Fock	insulator	0.3eV	ferro
experiment	slightly insulating (close to transition)	~ 0-0.15eV	AF? not well known
DFT-PIRG	close to transition (slightly insulating)	~ 0-0.1eV	nontrivial AF, stripe orbital plaquette spin order

experimental test?

Electronic structure of YVO_3

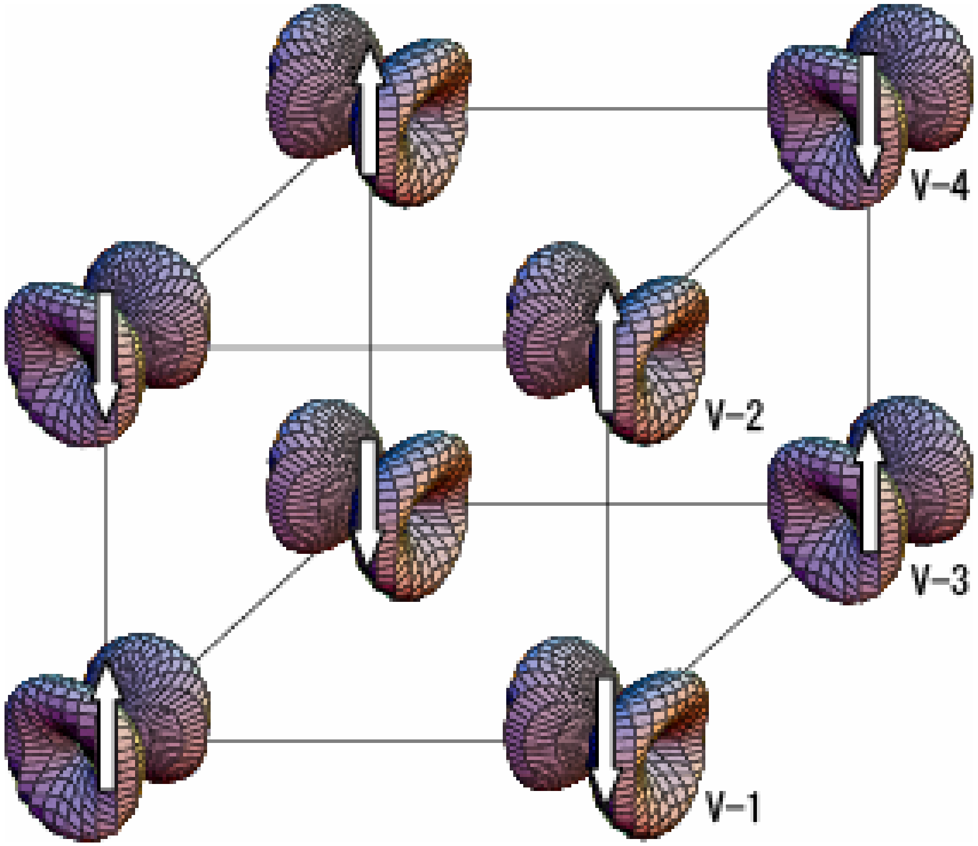


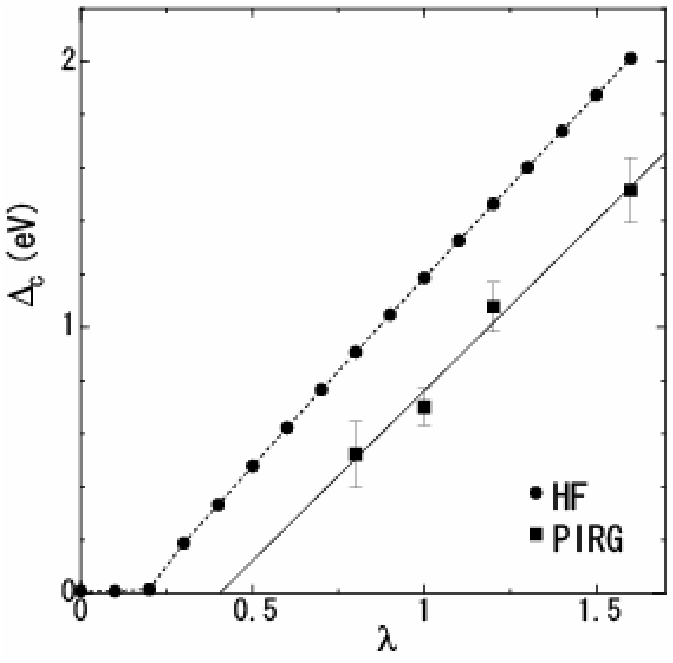


Otsuka

M. IMADA

Electronic structure of YVO_3





gap ~ 0.7 eV

Otsuka

Summary

Algorithm of Auxiliary-Field Path Integral for Fermions

PIRG; quantum number projection

Applications

Hubbard models; Mott transitions
quantum spin liquids

Realistic models; DFT+PIRG
downfolding + low-energy solver

Outlook

Convergence depends on lattice structure, interaction and system size

Local minimum