An Introduction to Quantum Monte Carlo for Strongly Correlated Electrons

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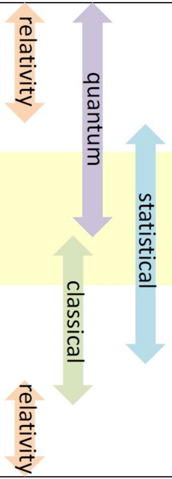
AICS Cafe (24/02/2012)

Outline

1. Background
   - target
   - model
   - methods
2. determinant QMC (det-QMC)
   - formulation
   - Example: 2d Hubbard model
3. Stochastic Series Expansion (SSE-QMC)
   - formulation
   - Example: 1d extended Hubbard model coupled to lattice
4. Summary

condensed matter physics

size (cm)	target	mechanics	category
10^{-33}	the early stages of the Big Bang		cosmology (gr-qc)
10^{-16}	weak interaction		particle physics
10^{-13}	atomic nucleus		nuclear physics
10^{-8}	atom		
10^{-7}	molecule		**cond-mat**
10^{-4}	DNA		
10^{0}	apple		biophysics
10^{2}	human		
10^{9}	earth		
10^{15}	solar system		astrophysics
10^{28}	universe		cosmology

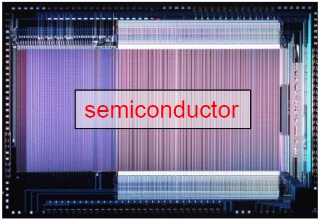


motivation

the 20st century

Bloch's theorem (1928)
→ Band theory

"free" electrons
(weekly correlated)



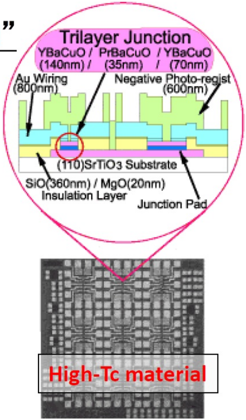
Next generation

"strongly correlated"

target materials

- transition metal oxide
- rare earth compound
- molecular conductors

etc...



strongly-correlated electron systems

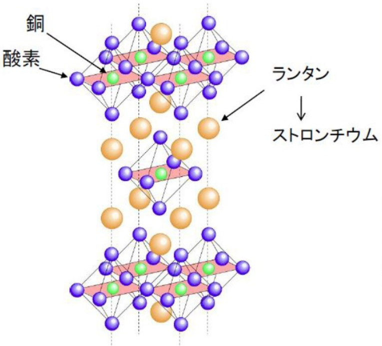
basic science:

- quantum many-body systems
- coupled degrees of freedom
  - charge, spin, orbital, lattice
- variety: phase transitions
  "More is different."
  P. W. Anderson (1967)
- challenging

applied physics:

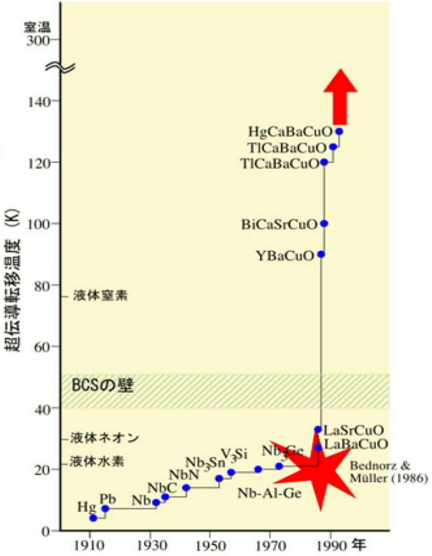
- High-Tc superconductivity
- magnetism
- ferroelectricity
- multiferroic
- material design / phase control

High-Tc fever in 1986



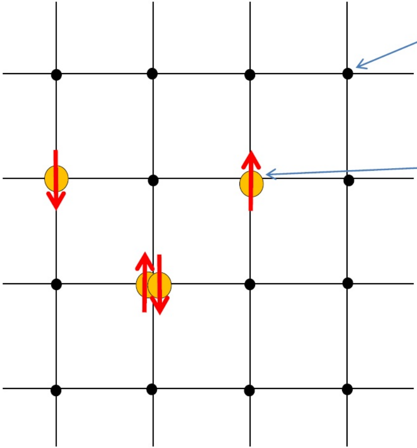
層状ペロブスカイト

CuO_2 平面



- doped Mott insulators

electrons in lattice: tight-binding model



"site":
outermost orbital / HOMO

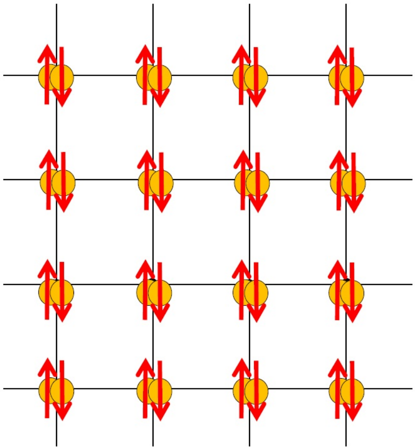
electron:
- charge (-e) & spin (↑ or ↓)
- Pauli exclusion principle

filling:
$n = Ne/N \leqq 2$

Ne: # of electrons
N : # of sites

"CuO2 plane"

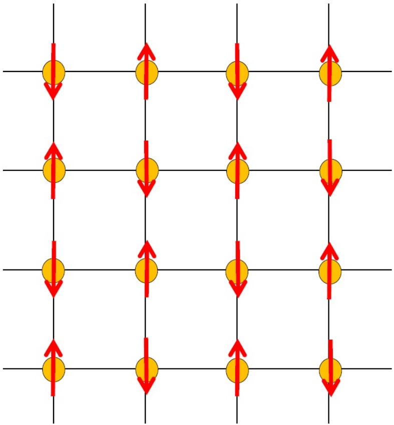
electrons in lattice: band insulator



n = Ne/N = 2

Insulating state
due to periodic potential

electrons in lattice: Mott insulator



n = Ne/N = 1

Insulating state
due to Coulomb interactions

canonical model: Hubbard model

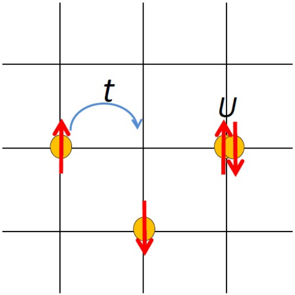
$$\mathcal{H} = \mathcal{H}_{\rm t} + \mathcal{H}_{\rm U}$$

$$\mathcal{H}_{\rm t} = -t \sum_{\sigma=\uparrow,\downarrow} \sum_{<i,j>} \left(c^{\dagger}_{i\sigma} c_{j\sigma} + c^{\dagger}_{j\sigma} c_{i\sigma} \right)$$

~ kinetic energy

$$\mathcal{H}_{\rm U} = U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

~ Coulomb repulsion



- "quantum"

$$\mathcal{H}_{\rm t}\mathcal{H}_{\rm U} \neq \mathcal{H}_{\rm U}\mathcal{H}_{\rm t}$$

- "many-body"

$$n_{i\uparrow} n_{i\downarrow} \neq n_{i\uparrow} \langle n_{i\downarrow} \rangle$$

parameters:

U/t, n, T/t

numerical methods for strongly-correlated electrons

- Exact Diagonalization (ED)
  - + "exact"
  - − only for small cluster ($N \sim 40$)
- Density Matrix Renormalization Group (DMRG)
  - + large system ($N \sim 1000$)
  - − only for 1D
- Quantum Monte Carlo (QMC)
  - + large system ($N \sim 1000$)
  - + $d > 1$
  - − negative sign problem

What is QMC ?

QMC = quantum-classical mapping + importance sampling

"quantum-classical mapping"

classical: $\langle A \rangle = \frac{1}{Z} \sum_n A_n e^{-\beta E_n}$

quantum: $\langle A \rangle = \frac{1}{Z} \sum_\alpha \langle \alpha | \hat{A} e^{-\beta \hat{H}} | \alpha \rangle$

Q: How to integrate out without diagonalization?

A: map to $(d+1)$ dim. classical system

"importance sampling"

$$\langle A \rangle = \frac{1}{Z} \sum_{\{c\}} A(\{c\}) W(\{c\})$$

$$Z = \sum_{\{c\}} W(\{c\})$$

- configuration: $\{c\} \sim 2^N$
- general method for high dimensional integrals

(roughly) 3 ways for quantum-classical mapping

1. world-line QMC (WL-QMC)
   - path-integral w/ checkerboard decomposition
   - electrons: only for 1d
   - spins: without frustration
2. Stochastic Series Expansion (SSE-QMC)
   - based on high-temperature series expansion
   - similar to WL-QMC
3. determinant QMC (det-QMC)
   - path-integral w/ Hubbard-Stratonovitch transformation
   - d $>$1

organization

determinant QMC

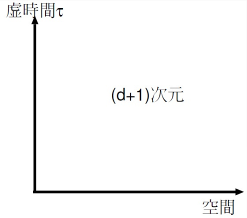
- procedure:
  - Suzuki-Trotter decomposion
  - Hubbard-Stratonovich transformation $\rightarrow \{s_{il}\}$: auxiliary field
  - Integrating out fermions
  - MC sampling for $\{s_{il}\}$
- example:
  - some results for 2d Hubbard model

Suzuki-Trotter decomposition

$$\begin{aligned} Z &= \mathrm{Tr}\ e^{-\beta\mathcal{H}} \\ &= \mathrm{Tr}\ e^{-L\Delta\tau(\mathcal{H}_t+\mathcal{H}_U)} \\ &\simeq \mathrm{Tr}\prod_{l=1}^{L} e^{-\Delta\tau\mathcal{H}_t} e^{-\Delta\tau\mathcal{H}_U} \end{aligned}$$

$$(\beta = L\Delta\tau)$$

- quantum-to-classical mapping
- d-dim. quantum system = $(d+1)$-dim. classical system



discrete Hubbard-Stratonovich transformation

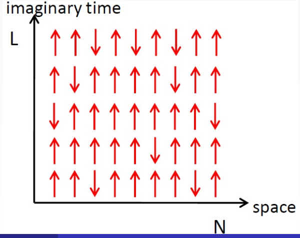
$$e^{-\Delta\tau U(n_{i\uparrow}-\frac{1}{2})(n_{i\downarrow}-\frac{1}{2})} = \frac{1}{2}e^{-\Delta\tau U/4}\sum_{s_{il}=\pm 1} e^{-\lambda s_{li}(n_{i\uparrow}-n_{i\downarrow})}$$

$\{s_{li}\}$: auxiliary field

$$\Rightarrow Z = \mathrm{Tr}_{\{s_{li}\}}\mathrm{Tr}_F \prod_{l=1}^{L} D_{\uparrow l} D_{\downarrow l}$$

$\mathrm{Tr}_{\{s_{li}\}}$: trace over Ising spins (2^{NL})

Tr_F: trace over free fermions



Trace out fermions

$$\mathrm{Tr}_F \prod_{l=1}^{L} D_{\uparrow l} D_{\downarrow l} = \det \mathcal{O}_\uparrow \det \mathcal{O}_\downarrow$$

$$\mathcal{O}_\sigma = \begin{pmatrix} I & 0 & \cdots & 0 & B_{\sigma 1} \\ -B_{\sigma 2} & I & 0 & \ldots & 0 \\ 0 & -B_{\sigma 3} & I & \ldots & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ 0 & \ldots\ldots & 0 & -B_{\sigma L} & I \end{pmatrix}$$

$$B_{\sigma l} = e^{-K} e^{-V_{\sigma l}} \quad : N \times N \text{ matrix}$$

$$\begin{aligned} \det \mathcal{O}_\sigma &= \det M_\sigma \\ M_\sigma &= I + B_{\sigma L} B_{\sigma L-1} \cdots B_{\sigma 1} \end{aligned}$$

$$\Rightarrow \quad Z = \mathrm{Tr}_{\{s_{li}\}} \det M_\uparrow \det M_\downarrow$$

physical observables: Green's function

$$\langle\langle c_{i\sigma} c^\dagger_{j\sigma} \rangle\rangle = \frac{1}{Z} \mathrm{Tr} \left(c_{i\sigma} c^\dagger_{j\sigma} e^{-\beta\mathcal{H}} \right) = \frac{\mathrm{Tr}_{\{s_{li}\}} \langle c_{i\sigma} c^\dagger_{j\sigma} \rangle \det M_\uparrow \det M_\downarrow}{\mathrm{Tr}_{\{s_{li}\}} \det M_\uparrow \det M_\downarrow}$$

$$\langle c_{i\sigma} c^\dagger_{j\sigma} \rangle = \frac{\mathrm{Tr}_F \, c_{i\sigma} c^\dagger_{j\sigma} \prod_{l=1}^{L} D_{\sigma l}}{\mathrm{Tr}_F \prod_{l=1}^{L} D_{\sigma l}} = (M_\sigma^{-1})_{ij}$$

MC sampling for configuration of Ising spins:

$$\langle\langle c_{i\sigma} c^\dagger_{j\sigma} \rangle\rangle = \lim_{N_{\mathrm{MC}} \to \infty} \frac{1}{N_{\mathrm{MC}}} \sum_{\mathrm{MC}} \langle c_{i\sigma} c^\dagger_{j\sigma} \rangle$$

with weight $W[\{s_{li}\}] = \det M_\uparrow \det M_\downarrow$

negative sign problem

- In general,
  W is <u>not</u> positive definite.
- some exceptions:
  - w/ p-h symmetry & bipartite lattice
- exponentially hard (?)
- Murphy's Law (?)

$$\langle\langle A\rangle\rangle = \frac{\sum_{\{s_{li}\}} \langle A\rangle W[\{s_{li}\}]}{\sum_{\{s_{li}\}} W[\{s_{li}\}]} = \frac{\sum_{\{s_{li}\}} \langle A\rangle \frac{W[\{s_{li}\}]}{|W[\{s_{li}\}]|} |W[\{s_{li}\}]|}{\sum_{\{s_{li}\}} \frac{W[\{s_{li}\}]}{|W[\{s_{li}\}]|} |W[\{s_{li}\}]|} = \frac{\sum_{\{s_{li}\}} \langle A\rangle \langle \mathrm{sgn}\, W[\{s_{li}\}]\rangle\, |W[\{s_{li}\}]|}{\sum_{\{s_{li}\}} \langle \mathrm{sgn}\, W[\{s_{li}\}]\rangle\, |W[\{s_{li}\}]|} = \frac{\langle\ \langle A\rangle\ \langle \mathrm{sgn}\, W[\{s_{li}\}]\rangle\ \rangle_{\mathrm{MC}}}{\langle\ \langle \mathrm{sgn}\, W[\{s_{li}\}]\rangle\ \rangle_{\mathrm{MC}}}$$

$$\langle \mathrm{sgn}\, W[\{s_{li}\}]\rangle = \frac{W[\{s_{li}\}]}{|W[\{s_{li}\}]|}$$

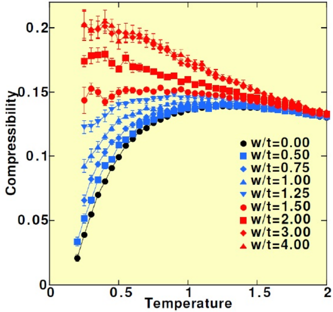
effect of randomness on Mott insulator

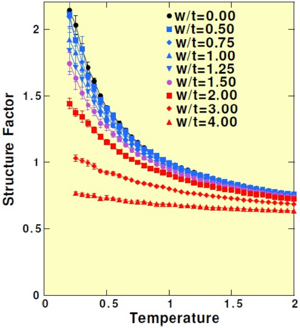
Anderson-Hubbard model

$$\mathcal{H} = -t \sum_{<j,k>,\sigma} \left(c_{j\sigma}^{\dagger} c_{k\sigma} + \mathrm{h.c.} \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + \sum_{i} \epsilon_i n_i$$

random potential

- Mott insulator: gapful, AF
- Anderson insulator: gapless, para





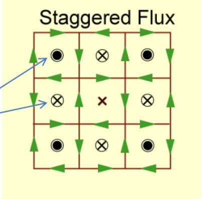
→ collapse of charge gap

YO, Y. Morita, Y. Hatsugai, PRB, 1998; J. Phys. Cond. Matt, 2000.

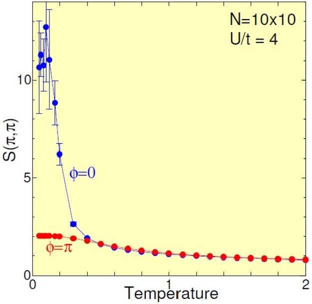
Hubbard model with staggered flux

$$\mathcal{H} = \sum_{<j,k>,\sigma} \left(c^\dagger_{j\sigma} t_{jk} c_{k\sigma} + c^\dagger_{k\sigma} t^*_{jk} c_{j\sigma} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

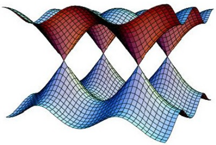
$$t_{jk} = t\, e^{i\theta_{jk}} \quad \Rightarrow \quad \phi \equiv \sum_{\text{plaquette}} \theta_{jk} = \pm\,\pi$$



“gauge field”
Affleck & Marston, PRB 1988.



suppression of AF due to flux



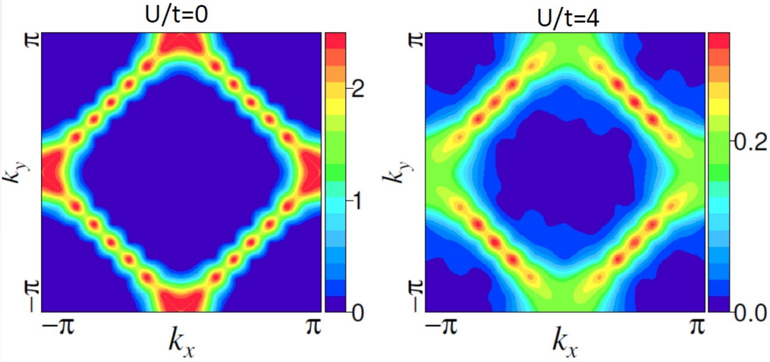
massless Dirac fermion

cf. graphene

YO, Y. Hatsugai, Phys. Rev. B (2002).

charge fluctuations in k-space

$$\kappa(\boldsymbol{k}) = \left.\frac{dn(\boldsymbol{k})}{d\mu}\right|_{\mu=0}$$



N=16x16, ∼100 MCS/1hour

YO, Y. Morita, Y. Hatsugai, Phys. Rev. B (2002).

organization

Stochastic Series Expansion

- procedure:
  - high-temperature series-expansion
  - truncation at fixed $L \to \{S_L\}$: operator string
  - graphical representation
  - MC sampling for $\{S_L\}$
- example:
  - 1d extended Hubbard model coupled to lattice

Heisenberg model

$$
\begin{aligned}
H &= J \sum_{<i,j>} \left\{ \Delta S_i^z S_j^z + \left(S_i^x S_j^x + S_i^y S_j^y \right) \right\} \\
&= J \sum_{<i,j>} \left\{ \Delta S_i^z S_j^z + \frac{1}{2} \left(S_i^+ S_j^- + S_i^- S_j^+ \right) \right\}
\end{aligned}
$$

base: $|\alpha\rangle = |\sigma_1 \sigma_2 \sigma_3 \cdots \sigma_N\rangle, \quad \sigma_i = \uparrow, \downarrow$

$$
\begin{aligned}
S_i^z | \uparrow_i \rangle &= | \uparrow_i \rangle & \qquad S_i^z | \downarrow_i \rangle &= | \downarrow_i \rangle \\
S_i^+ | \uparrow_i \rangle &= 0 & \qquad S_i^+ | \downarrow_i \rangle &= | \uparrow_i \rangle \\
S_i^- | \uparrow_i \rangle &= | \downarrow_i \rangle & \qquad S_i^- | \downarrow_i \rangle &= 0
\end{aligned}
$$

(1): Write H as a sum of bond operators

$$H = -\sum_{a=1}^{2}\sum_{b=1}^{M} H_{a,b}$$

a : operator type (1=diagonal, 2=off-diagonal)

b : bond index (b connects i(b) and j(b))

$$H_{1,b} = C - \Delta S^z_{i(b)} S^z_{j(b)}, \quad C > \Delta/4 \text{ : constant}$$

$$H_{2,b} = \frac{1}{2}\left(S^+_{i(b)} S^-_{j(b)} + S^-_{i(b)} S^+_{j(b)}\right)$$

(2): high-temperature series-expansion

$$
\begin{aligned}
Z &= \mathrm{Tr}\left\{e^{-\beta H}\right\} \\
&= \sum_{\alpha} \langle \alpha | e^{-\beta H} | \alpha \rangle \\
&= \sum_{\alpha} \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \langle \alpha | H^n | \alpha \rangle \\
&= \sum_{\alpha} \sum_{n=0}^{\infty} \sum_{S_n} \frac{\beta^n}{n!} \langle \alpha | H_{l_1} H_{l_2} H_{l_3} \cdots H_{l_n} | \alpha \rangle
\end{aligned}
$$

l_j : (a, b)

S_n : $[l_1, l_2, \cdots, l_n]$ (operator string)

(3): truncate at $n = L$

$$Z \simeq \sum_{\alpha} \sum_{n=0}^{L} \sum_{S_n} \frac{\beta^n}{n!} \langle \alpha | \prod_{l_j} H_{l_j} | \alpha \rangle$$

$$\because \quad \langle n \rangle = -\beta \langle H \rangle \text{ (finite lattice)}$$

(4): insert unit operators

$$Z = \sum_{\alpha} \sum_{S_L} \frac{\beta^n (L-n)!}{L!} \langle \alpha | \prod_{l_j=1}^{L} H_{l_j} | \alpha \rangle$$

$$l_j : \quad 0 \;\text{ or }\; (a, b)$$

$$H_0 = I$$

(5): physical observable

$$
\begin{aligned}
\langle A\rangle &= \frac{1}{Z}\mathrm{Tr}\left\{Ae^{-\beta H}\right\} \\
&= \frac{1}{Z}\langle\alpha|Ae^{-\beta H}|\alpha\rangle \\
&= \frac{1}{Z}\sum_{\alpha}\sum_{S_L}\frac{\beta^n(L-n)!}{L!}\langle\alpha|A\prod H_{l_j}|\alpha\rangle \\
&= \frac{1}{Z}\sum_{\alpha}\sum_{S_L}\frac{\langle\alpha|A\prod H_{l_j}|\alpha\rangle}{\langle\alpha|\prod H_{l_j}|\alpha\rangle}\cdot\frac{\beta^n(L-n)!}{L!}\langle\alpha|\prod H_{l_j}|\alpha\rangle \\
&= \frac{\sum_{\alpha}\sum_{S_L}A(\alpha,S_L)\,W(\alpha,S_L)}{\sum_{\alpha}\sum_{S_L}W(\alpha,S_L)}
\end{aligned}
$$

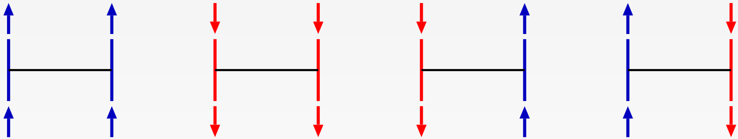
importance sampling for configuration $(\alpha, S_L) \Rightarrow$ MC

graphical representation for verteices

$$W(\alpha, S_L) = \frac{\beta^n (L-n)!}{L!} \langle \alpha(L)|H_{l_L}|\alpha(L-1)\rangle \cdots \langle \alpha(2)|H_{l_2}|\alpha(1)\rangle \cdot \langle \alpha(1)|H_{l_1}|\alpha(0)\rangle$$

diagonal operator: $H_{1,b}$

$\langle \uparrow\uparrow | H_{1,b} | \uparrow\uparrow \rangle$ $\langle \downarrow\downarrow | H_{1,b} | \downarrow\downarrow \rangle$ $\langle \uparrow\downarrow | H_{1,b} | \uparrow\downarrow \rangle$ $\langle \downarrow\uparrow | H_{1,b} | \downarrow\uparrow \rangle$



off-diagonal operator: $H_{2,b}$

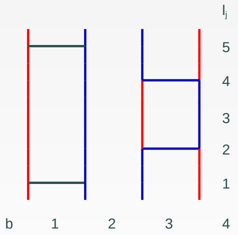
$\langle \uparrow\downarrow | H_{2,b} | \downarrow\uparrow \rangle$ $\langle \downarrow\uparrow | H_{2,b} | \uparrow\downarrow \rangle$

graphical representation for operator string

$$W(\alpha, S_L) = \frac{\beta^n (L-n)!}{L!} \langle \alpha(L) | H_{l_L} | \alpha(L-1) \rangle \cdots \langle \alpha(2) | H_{l_2} | \alpha(1) \rangle \cdot \langle \alpha(1) | H_{l_1} | \alpha(0) \rangle$$

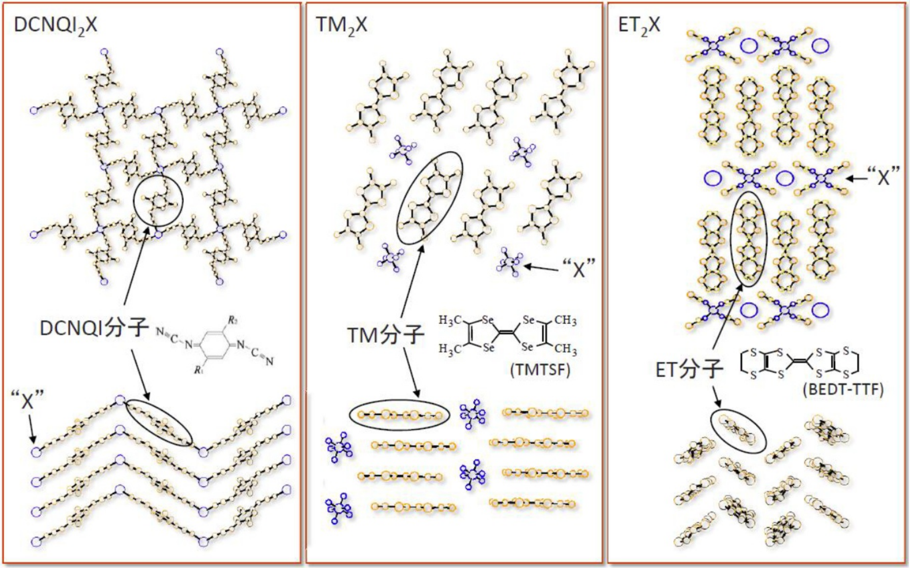
Ex. 4-site case:

$$N = 4$$
$$L = 5$$
$$|\alpha(0)\rangle = |\downarrow\uparrow\uparrow\downarrow\rangle$$
$$S_L = (H_{1,1}, H_{2,3}, H_{0,0}, H_{2,3}, H_{1,1})$$

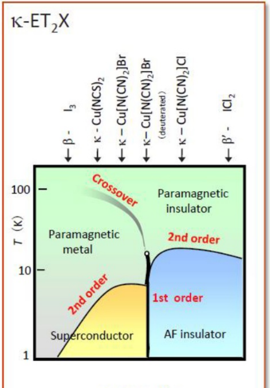


⇒ operator string: world-line (doubly linked list)

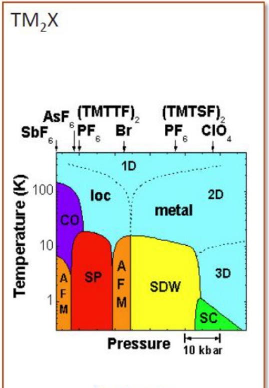
Molecular conductor: 1D π-electron system



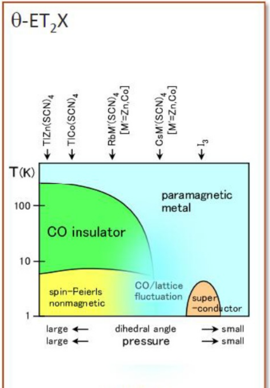
Molecular conductor: “colorful” phase diagrams



K. Kanoda



D. Jerome

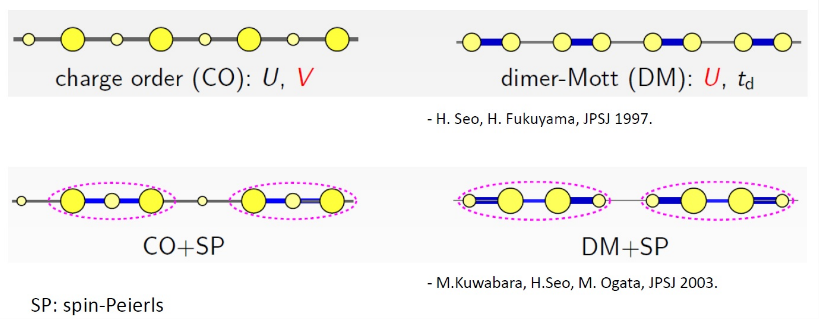


H. Mori

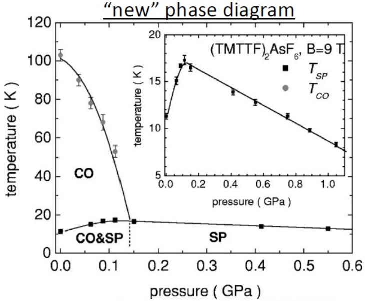
similar one-electron band structures but variety of properties
$\rightarrow$ interactions are important !

Molecular conductor: "colorful" phase diagrams

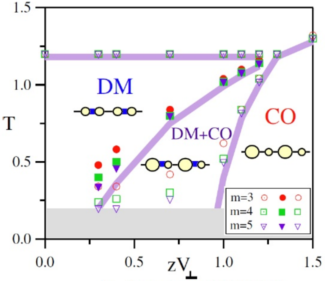
- "soft" → electron-lattice coupling, pressure
- low dimensinality → quantum/thermal flustuations
- clean & material design → "model" material



Molecular conductor: new phase diagram



Zamborszky *et al.*, PRB 2002.



H. Seo *et al.*, JPSJ 2007.

$$\hat{H} = \hat{H}_{\mathrm{extHub}} + \hat{H}_{\mathrm{e\text{-}l}} + \hat{H}_{\perp}$$

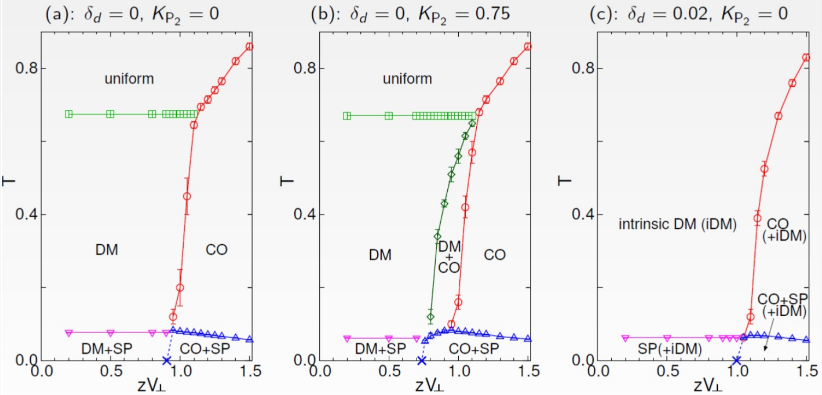
$$\hat{H}_{\mathrm{extHub}} = -\sum_{i,\sigma} t_i \left(c^{\dagger}_{i\sigma} c_{i+1\sigma} + \mathrm{h.c.} \right) + \sum_i U n_{i\uparrow} n_{i\downarrow} + \sum_i V n_i n_{i+1}$$

$$\hat{H}_{\mathrm{e\text{-}l}} = -\sum_{i,\sigma} t_i u_i \left(c^{\dagger}_{i\sigma} c_{i+1\sigma} + \mathrm{h.c.} \right) + \frac{K_{\mathrm{P}}}{2} \sum_i u_i^2 + \frac{K_{\mathrm{P_2}}}{4} \sum_i u_i^4$$

$$\hat{H}_{\perp} = V_{\perp} \sum_{\langle j,k \rangle} n_i^j n_i^k$$

- ¼-filled extended Hubbard model
- electron-lattice coupling
- inter-chain interaction

Molecular conductor: finite-T phase diagram



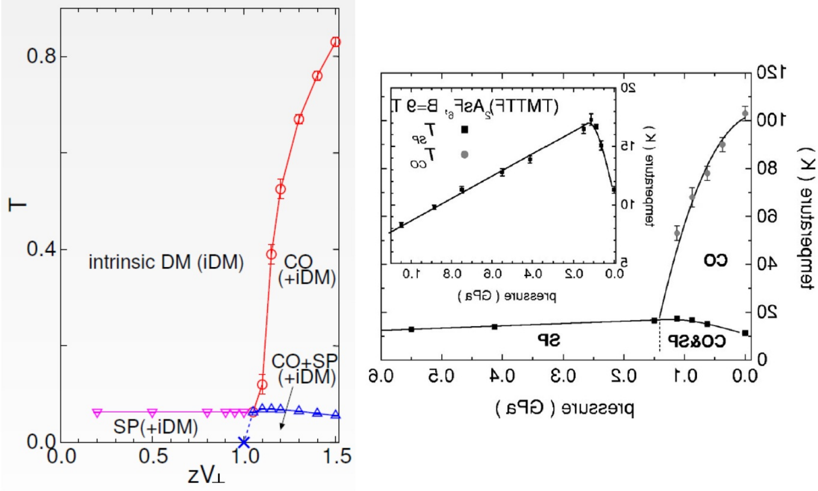
CO v.s. DM

CO+DM
→ ferroelectoricity

cf. TMTTF-salt

YO, H.Seo, T. Kato, Y. Motome (JPSJ 2008, Physica B 2008).

Molecular conductor: comparison with experiments



YO, H.Seo, T. Kato, Y. Motome (JPSJ 2008, Physica B 2008).

Summary

1. determinant QMC
   - procedure:
     - Trotter decomposion.
     - Hubbard-Stratonovich transformation $\rightarrow \{s_{il}\}$: auxiliary field
     - Integrating out fermions
     - MC sampling for $\{s_{il}\}$
   - example: 2d Hubbard model
2. Stochastic Series Expansion
   - procedure:
     - high-temperature series-expansion
     - truncation at fixed $L \rightarrow \{S_L\}$: operator string
     - graphical representation
     - MC sampling for $\{S_L\}$
   - example: 1d extended Hubbard model coupled to lattice