第12回学習物理領域セミナー＋第64回DLAP

Fermi Machine

Nov. 28, 2024

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Acknowledgements
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Shiro Sakai

何が問題か？

量子多体問題の基底状態：　$H\left|\Psi_0\right\rangle = E_0\left|\Psi_0\right\rangle$

$\left|\Psi_0\right\rangle = \sum_n c_n \left|\varphi_n\right\rangle$　N粒子(Nサイト)系のヒルベルト空間 $e^{\alpha N}$；

NPハード問題

系統的に精度を向上させられるアルゴリズムで
多項式時間(メモリ)$\propto N^\beta$の範囲で、
如何にうまく基底状態を近似し、新しい物理を明らかにするか？

波及効果
物理学（高エネルギー、原子核、物性）、化学、生物学、
種々の工学的課題

既存の量子系の数値計算手法のあれこれ

量子モンテカルロ法

Feynman path integral

$$Z = \mathrm{Tr}\exp[-\beta H] = \sum_x \langle x | \exp[-\beta H] | x \rangle$$

負符号問題

変分波動関数法 — 基底状態や励起状態波動関数を求める

密度行列繰込み群DMRG
テンソルネットワーク
変分モンテカルロ(VMC)
などなど

最近, ボルツマンマシン, CNN, transformer などの人工NNの開発が急速

変分不等式

$$E_g \le \frac{\langle \Phi_\alpha | H | \Phi_\alpha \rangle}{\langle \Phi_\alpha | \Phi_\alpha \rangle}$$

強い多体相関（強相関）や量子もつれを伴うチャレンジ課題をいかにうまく扱うか？
機械学習はどんな貢献ができるか？

Outline

J. Phys. Soc. Jpn. 93, 104002 (2024)

機械学習（人工NN）を用いた全く新しい量子多体ソルバーの開発

1.既存のBoltzmann machine, CNN, transformerなどでは
隠れ変数としてほとんど, イジング変数等の古典変数を採用している.
その代わりに隠れ変数としてフェルミオンを採用し,
「フェルミマシン」を構築する.

2. フェルミマシンのアルゴリズムに, 銅酸化物等で実験検証が進む
電子の分数化の概念と理解を実体化することで,
強相関多体フェルミオンの示す創発構造を予め具現化して利用し,
量子もつれを効率的に取り込むことを狙う.

Introduction

既存のNN変分波動関数の例：RBMによる波動関数の表現

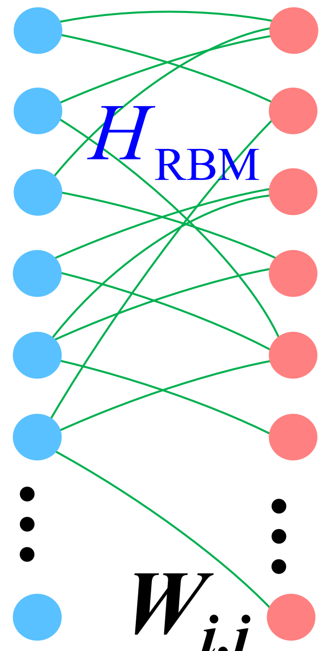
Carleo, Troyer, Science 355, 602 (2017)

Example; spin-1/2 Heisenberg model

$$H=\sum_{i,j} J_{i,j}\boldsymbol{S}_i\cdot\boldsymbol{S}_j$$

$$H_{\rm RBM}=\sum_i a_i S_i^z+\sum_{i,j} W_{i,j}S_i^z h_j+\sum_j b_j h_j$$

physical variables S_i^z



hidden variables h_j

b

h_j：擬イジングスピン(binary)

$Z_S=\mathrm{Tr}_h\exp[-\beta_{\rm RBM}H_{\rm RBM}]$　ボルツマン重み

部分対角和を取った分配関数→基底状態波動関数の重み

$$Z_S=\exp[-a_i\beta_{\rm RBM}S_i^z]\prod_k 2\cosh\left[\beta_{\rm RBM}(b_k+\sum_i W_{ik}S_i^z)\right]\to\mathcal{N}$$

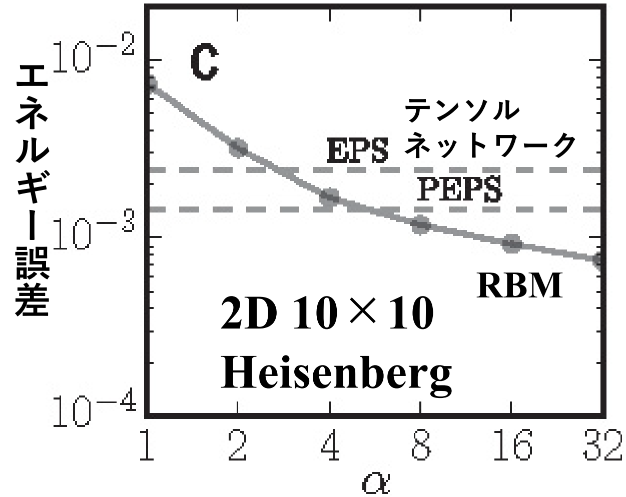
$|\Psi\rangle=\mathcal{N}\sum_y|y\rangle,$ 量子もつれのない単純な等分配状態(温度∞状態)に作用させる

$\alpha=\{a,\ b,\ W\}$; 変分パラメタ

Hの期待値 $\langle H\rangle=\langle\Psi|H\sum_x|x\rangle\langle x|\Psi\rangle/\langle\Psi|\Psi\rangle$

を下げるように $a,\ b,\ W$ を訓練する

→ 甘利による自然勾配法を用いる。



$$\alpha=\frac{\text{隠れ変数の数}}{\text{物理変数の数}}$$

MC sampling

$\boldsymbol{x}=\{S_1^z,S_2^z,\ldots\ldots S_N^z\}$

チャレンジである遍歴電子系やフラストレーションのあるスピン系では精度に限界

従来の変分波動関数による基底状態表現の例, VMC

Gross, Sorella, Tahara & Imada

$$|\psi\rangle = \mathcal{L}_L \, \mathcal{P}_{\rm J} \mathcal{P}^{\rm ex.}_{\rm d\text{-}h} \mathcal{P}_{\rm G} \, \mathcal{L}^{S=0} \, |\phi_{\rm pair}\rangle$$

$$\left|\phi_{\text{pair-product}}\right\rangle = \left[\sum_{ij} f_{ij} c^{\dagger}{}_{i\sigma} c^{\dagger}{}_{j\sigma'}\right]^{N/2} |0\rangle$$

pair-product (ペア積)
geminal　；量子化学
HFB　；原子核

Gutzwiller factor

$$\mathcal{P}_{\rm G} = \exp\left[-g \sum_i n_{i\uparrow} n_{i\downarrow}\right]$$

long-ranged Jastrow factor

$$\mathcal{P}_{\rm J} = \exp\left[-\frac{1}{2} \sum_{i \neq j} v_{ij} n_i n_j\right]$$

quantum number projection

$$\mathcal{L}^S = \frac{2S+1}{8\pi^2} \int d\Omega \, P_S(\cos\beta) \hat{R}(\Omega)$$

spin, momentum, point group….

cf. 原子核計算

Open source: mVMC

Comput. Phys. Commun. 235, (2019) 447

Combined VMC and Neural Network

Nomura, Darmawan, Yamaji, Imada
PRB 96, 205152 (2017)

ペア積波動関数+ RBM

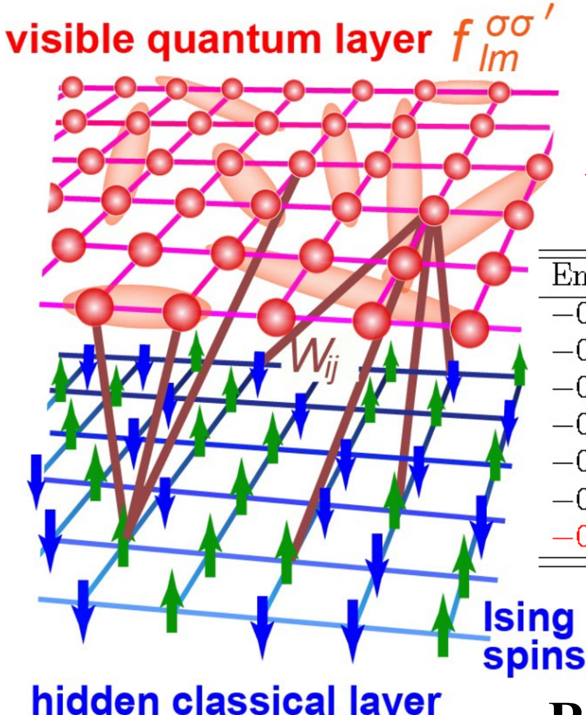
Pfaffian

$$|\Psi\rangle = \mathcal{P}\mathcal{L}^{K=0}\mathcal{L}^{C_4}\mathcal{N}\sum_x |x\rangle\overbrace{\langle x|\mathcal{L}^{S=0}|\phi_{\text{pair-product}}\rangle}^{\text{Pfaffian}}$$ **RBM+PP**

$$|\phi_{\text{pair-product}}\rangle = \left[\sum_{ij} f_{ij} c^{\dagger}_{i\sigma} c^{\dagger}_{j\sigma'}\right]^{N/2} |0\rangle$$

量子もつれの取り込み
node構造の最適化
系統的改良の可能性

RBM+PP architecture



$$\mathcal{N} = \prod_k 2\cosh(\beta(b_k + \sum_i W_{ik} S_i^z))$$

$$\mathcal{N} = \prod_{k,\sigma} 2\cosh(\beta(b_k + \sum_i W_{i\sigma k}(2n_{i\sigma} - 1)))$$

b, W, f ; variational parameter
S, n ; physical variable

Energy per site	Wave function	Reference
−0.494757(12)	Neural quantum state	Szabo *et al.*(2020)
−0.49516(1)	CNN	Choo *et al.* (2019)
−0.49521(1)	VMC(p=0)	Hu *et al.* (2013)
−0.495530	DMRG	Gong *et al.* (2014)
−0.49575(3)	RBM-fermionic w.f.	Ferrari *et al.* (2019)
−0.497549(2)	VMC(p=2)	Hu *et al.* (2013)
−0.497629(1)	RBM+PP	present study

フラストレーションの大きい正方格子J_1-J_2ハイゼンベルク模型（$J_2/J_1 = 0.5$）のベンチマーク

NNが強結合超伝導やスピン液体などの挑戦課題の解明に使える実用最高レベルの精度に

RBM+PPを実装したVMCオープンソースコード

mVMC

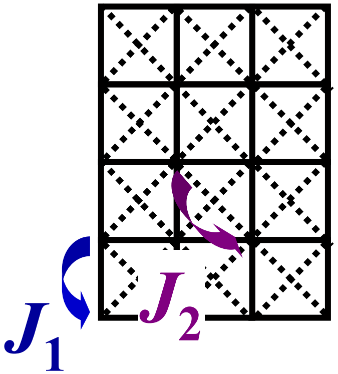
https://github.com/issp-center-dev/mVMC/releases/tag/v1.3.0

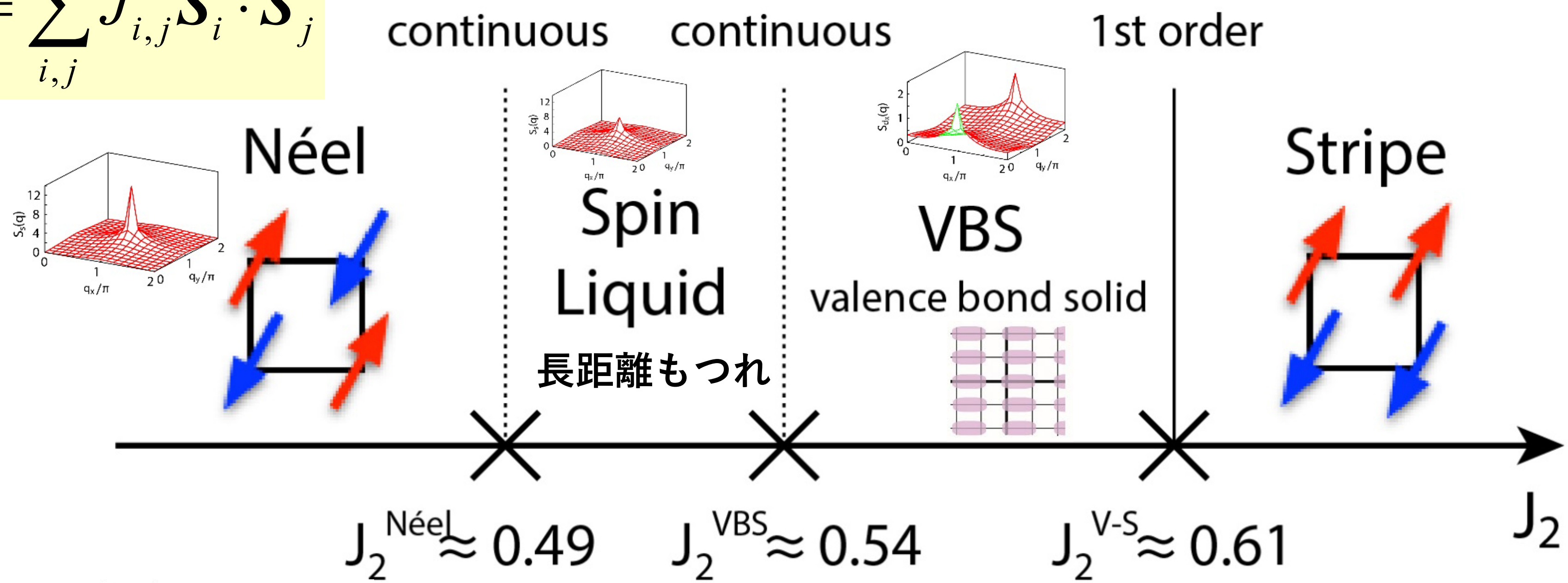
IMADA

Fractionalization in J_1-J_2 model

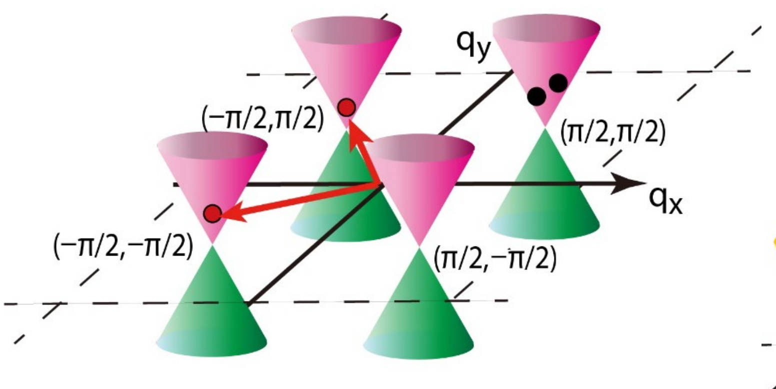
Y. Nomura, M. Imada, PRX, 11, 031034 (2021)

$$H = \sum_{i,j} J_{i,j} \boldsymbol{S}_i \cdot \boldsymbol{S}_j$$

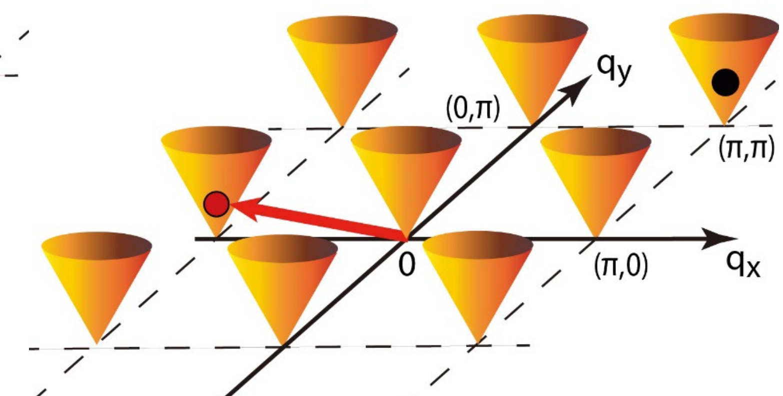




spinon excitation



spin excitation



基本励起がスピン
ではなく
スピンが分裂した
スピノンで表される。

Neural network for quantum many-body solver

However,….
hidden variables in RBM are so far classical (Ising spins).
If hidden variables are quantized and replaced by fermions,
they may represent fermionic entanglement and
node structure more efficiently.

To implement the correlation effects in the Fermi machine,
a key concept is the fermion fractionalization,
where strong correlation splinters a fermion (electron)
into entangled emergent multi-fermions.

$$H_{\mathrm{TCFM}} = \sum_{k}\left[\varepsilon_c(k) c^{\dagger}_{k\sigma} c_{k\sigma} + \varepsilon_d(k) d^{\dagger}_{k\sigma} d_{k\sigma}\right] + \sum_{k,\sigma} \Lambda(k)\left(c^{\dagger}_{k\sigma} d_{k\sigma} + \mathrm{H.c.}\right)$$

This fractionalization has experimental & theoretical supports
indeed in the cuprate superconductors.

Hidden variables representing the entanglement/correlation
should be related to the fermionic self-energy representation.

カギとなるコンセプトはどんな分数化か？

分数化のいろいろ
１次元系のスピン電荷分離　**Tomonaga, Luttinger**
ハドロン↔クォーク　**Gell-Mann, Zweig, Ne`eman**
ポリアセチレンソリトン　**SSH**
分数量子ホール効果　**Laughlin, Jain….**
スレーブボソン、スレーブフェルミオン
Kotliar, Ruckenstein, Sachdev…..

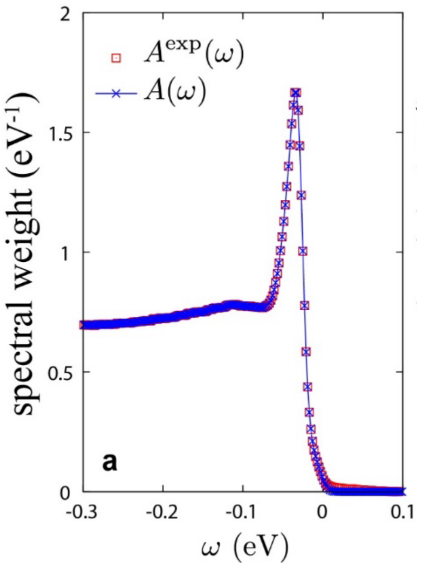
どれとも異なる新奇な分数化：
１つのフェルミオンから複数のフェルミオンが創発

Signature of Fractionalization: Structure of Self-Energy in SC State

1電子グリーン関数 $G(k,\omega)=\dfrac{1}{\omega-\varepsilon_0(k)-\Sigma(k,\omega)}$

Σ；自己エネルギー

Interaction effect



$$A(k,\omega)=-\frac{1}{\pi}\mathrm{Im}\,G(k,\omega)$$ スペクトル関数：観測可能

ARPES data

角度分解光電子分光

Kondo *et al.* Nat. Phys. 7, 21 (2011)

超伝導状態

$$G_{11}^{\mathrm{nor}}(\mathbf{k},\omega)=\left[\omega+\mu-\varepsilon_{\mathbf{k}}-\left(\Sigma^{\mathrm{nor}}(\mathbf{k},\omega)+W(\mathbf{k},\omega)\right)\right]^{-1}$$

$$W(\mathbf{k},\omega)=\frac{\Sigma^{\mathrm{ano}}(\mathbf{k},\omega)^2}{\omega-\mu+\varepsilon_{\mathbf{k}}+\Sigma^{\mathrm{nor}}(\mathbf{k},-\omega)^*}$$

***W*; interaction effect from superconducting part**

$A(k,\omega)\rightarrow\Sigma^{\mathrm{nor}},\Sigma^{\mathrm{ano}}$ を別々に抽出；逆問題

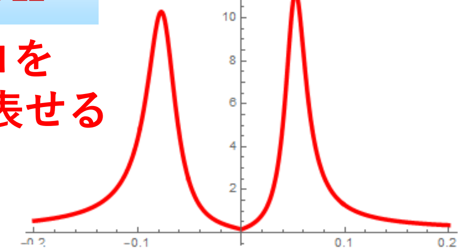
M. IMADA

Prediction by fractionalization: Self-energy peak cancellation

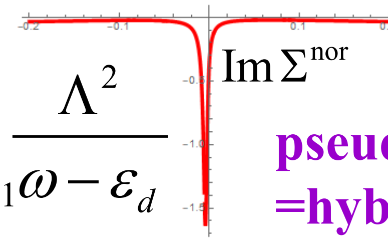
$$H_{\mathrm{TCFM}} = \sum_k \left[\varepsilon_c(k) c^\dagger_{k\sigma} c_{k\sigma} + \varepsilon_d(k) d^\dagger_{k\sigma} d_{k\sigma} \right] + \sum_{k,\sigma} \Lambda(k) \left(c^\dagger_{k\sigma} d_{k\sigma} + \mathrm{H.c.} \right)$$

Gのゼロを容易に表せる

$$G_c = \frac{1}{(\omega - \varepsilon_c) - \Sigma^{\mathrm{nor}}(\mathbf{k},\omega)}$$



$$A(k,\omega) = -\frac{1}{\pi} \mathrm{Im}\, G^{\mathrm{nor}}(k,\omega)$$



$$\Sigma^{\mathrm{nor}}(\mathbf{k},\omega) = \frac{\Lambda^2}{\omega - \varepsilon_d}$$

How about SC?

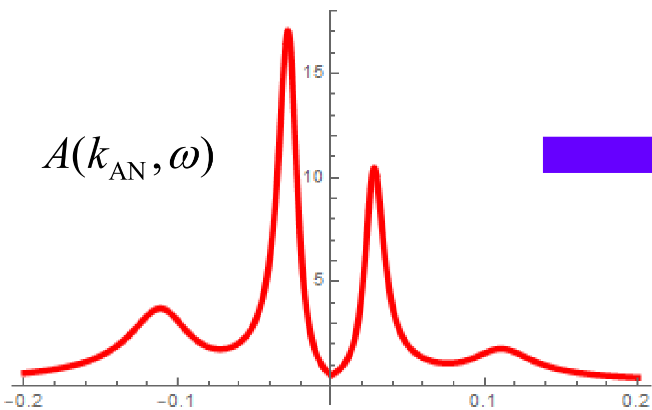
Sakai, Civelli, Imada PRL 116, 057003 (2016)

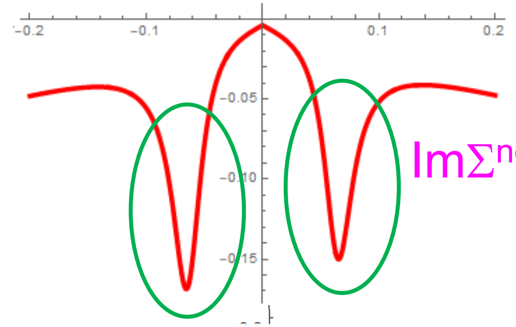
Extension of TCFM to SC phase

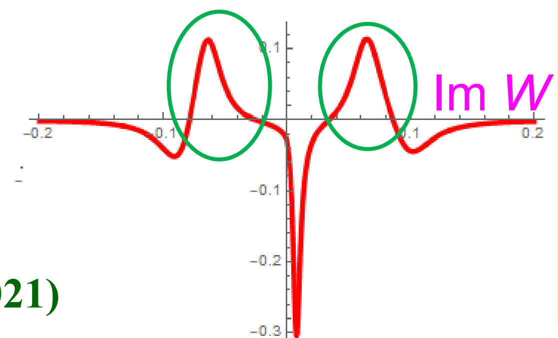
$$G_c^{\mathrm{nor}}(\mathbf{k},\omega) = \left[\omega + \mu - \varepsilon_{\mathbf{k}} - \left(\Sigma^{\mathrm{nor}}(\mathbf{k},\omega) + W(\mathbf{k},\omega) \right) \right]^{-1}$$

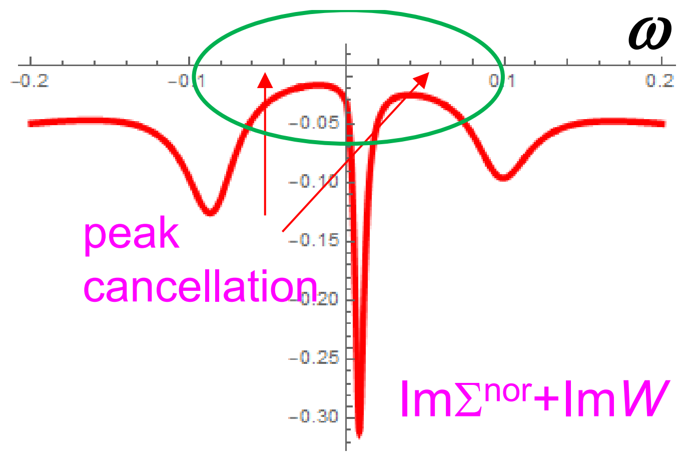
$$W(\mathbf{k},\omega) = \frac{\Sigma^{\mathrm{ano}}(\mathbf{k},\omega)^2}{\omega - \mu + \varepsilon_{\mathbf{k}} + \Sigma^{\mathrm{nor}}(\mathbf{k},-\omega)^*}$$

pseudogap
=hybridization gap
⇒銅酸化物擬ギャップ







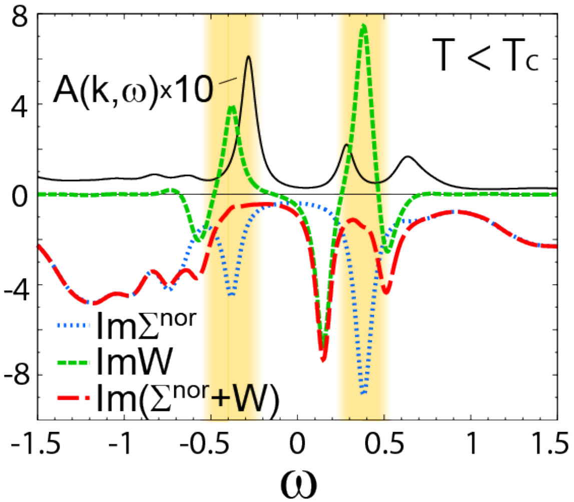


Prominent peaks emerge in ImΣ$^{\mathrm{nor}}$ and ImΣ$^{\mathrm{ano}}$ and Im Σ$^{\mathrm{ano}}$ peak generates SC. but they cancel in $A(k,\omega)$: Fingerprint of fractionalization

Imada, Suzuki, JPSJ 88, 024701 (2019)
Imada J. Phys. Soc. Jpn. 90, 074702 (2021)

Indications of electron fractionalization in theories and experiments

1. cluster DMFT for SC Hubbard: Cancellation of normal and anomalous contributions to spectral function $A(k,\omega)$;

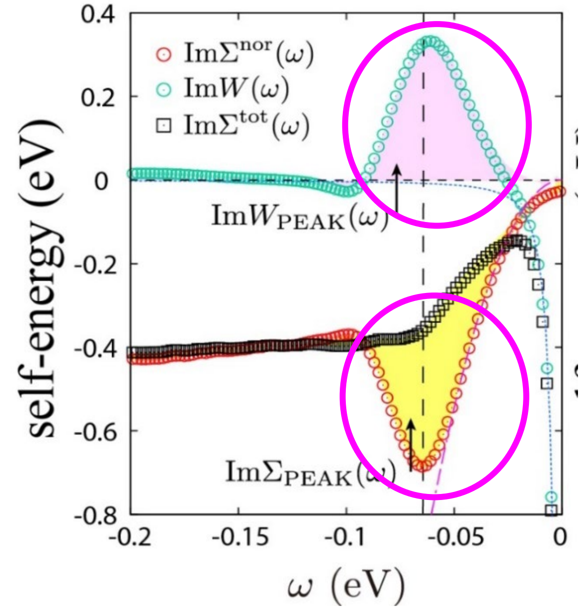


分数化に特有の性質

⇦ Sakai *et al.* (2016)

Yamaji *al.* (2021) ➡

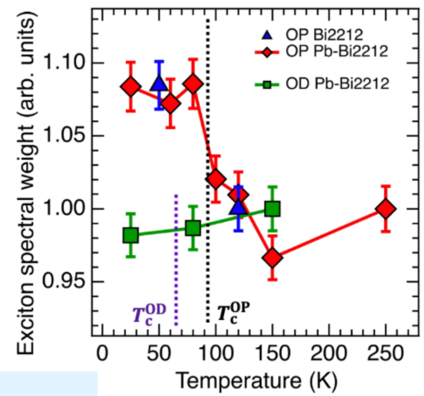
隠れたフェルミオンの
存在の示唆



2. Same cancellation inferred from machine learning of cuprate ARPES

3. RIXS data supporting fractionalization

Imada (2021)
Singh *et al.* (2022) ➡



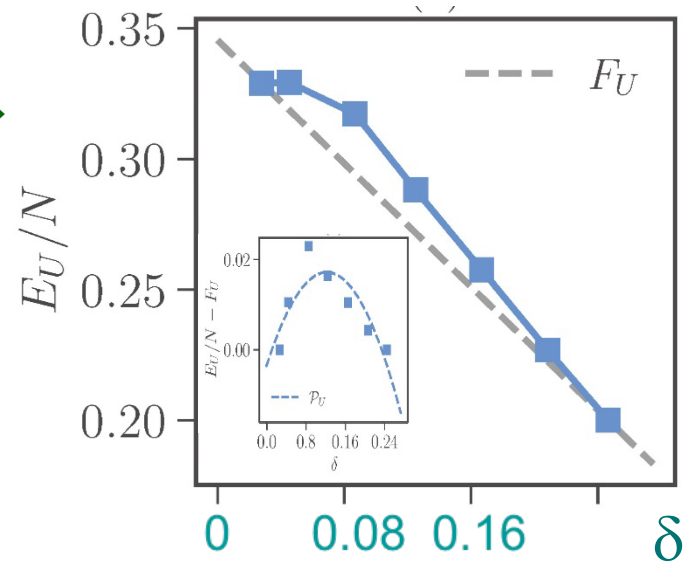
Two component fermion model (TCFM)

$$H = \sum_k [\varepsilon_c(k) c_{k\sigma}{}^{\dagger} c_{k\sigma} + \Lambda_k (c_{k\sigma}{}^{\dagger} d_{k\sigma} + \mathrm{H.c.}) + \varepsilon_d(k) d_{k\sigma}{}^{\dagger} d_{k\sigma}]$$

Origin of electron fractionalization

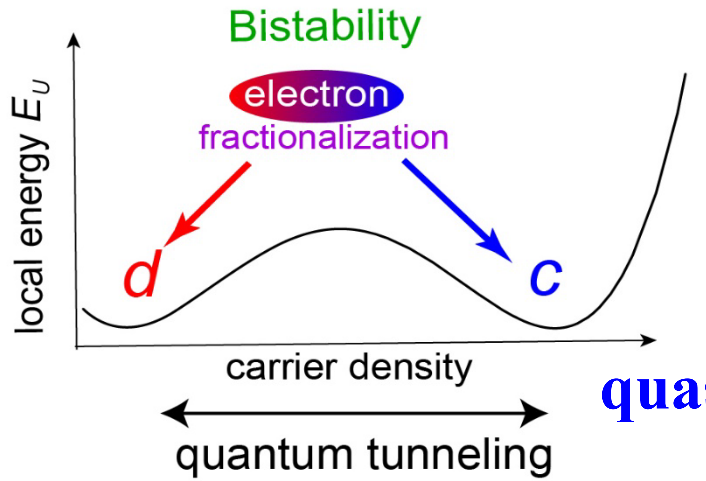
Ab initio **studies of cuprates:**
局所斥力によって分数化と局所有効引力が創発する

Schmid *et al.* (2023) ➡



$$E_U = U\left\langle n_{i\uparrow} n_{i\downarrow} \right\rangle$$

dark fermion *d*
= detected as
incoherent part
of electron



quasiparticle

1成分強相関電子の*c*と*d*への分数化

TCFM
$$H = \sum_k [\varepsilon_c(k) c_{k\sigma}^\dagger c_{k\sigma} + \Lambda_k (c_{k\sigma}^\dagger d_{k\sigma} + \mathrm{H.c.}) + \varepsilon_d(k) d_{k\sigma}^\dagger d_{k\sigma}]$$

New fractionalization picture
Fractionalization of a fermion into two fermions associated with trend to 1st-order transition; phase separation replaced by quantum resonant, entangled and spatially uniform state stabilized by quantum tunneling

cf. **slave boson, slave fermion; Kotliar-Ruckenstein, Lee-Nagaosa, Read-Sachdev**

What is fractionalization? How to materialize?

Zhu, Zhu PRB 87, 085120 (2013), Sakai *et al.* PRB 94, 115130 (2016)

$$\mathcal{H} = U n_\sigma n_{-\sigma}$$

Hubbard in the atomic limit (1-site Hubbard)

$$n_\sigma = c_\sigma^\dagger c_\sigma$$

Two-component fermion model (TCFM)

$$\tilde{c}_\sigma \doteq c_\sigma$$

$$\tilde{d}_\sigma \doteq c_\sigma (1 - 2n_{c-\sigma})$$

$$H = \sum_\sigma [\mu_{\tilde{c}} \tilde{c}_\sigma^\dagger \tilde{c}_\sigma + \mu_{\tilde{d}} \tilde{d}_\sigma^\dagger \tilde{d}_\sigma + \Lambda(\tilde{c}_\sigma^\dagger \tilde{d}_\sigma + h.c)]$$

$$\mu_{\tilde{c}} = \mu_{\tilde{d}} = -\Lambda = \frac{U}{2}$$

$$-\tilde{c}_\sigma^\dagger \tilde{d}_\sigma = -c_\sigma^\dagger c_\sigma (1 - 2n_{-\sigma})$$
$$= -n_\sigma + 2 n_\sigma n_{-\sigma}$$

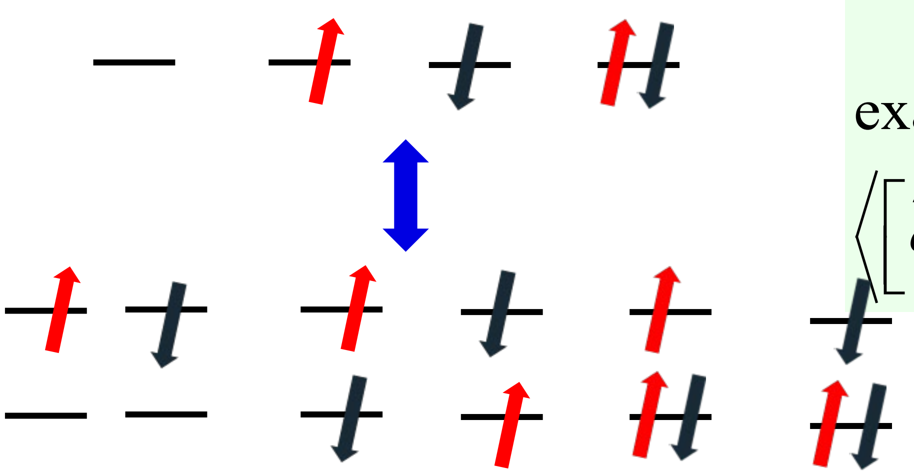
$\tilde{d}_\sigma$ is identified as the dark fermion

$\tilde{c}, \tilde{d}$: fermion operator,

orthogonal as an average at half filling $\langle n_\sigma \rangle = 1$:

exact fermion anticommutation of $\tilde{c}$ and $\tilde{d}$

$$\left\langle \left[\tilde{c}, \tilde{d}^\dagger \right]_+ \right\rangle = 0, \quad \left\langle \left[\tilde{d}, \tilde{d}^\dagger \right]_+ \right\rangle = 1, \; .....$$



Restrict Hilbert space within n=1,2,3 for TCFM.

Mott gap interpreted by TCFM

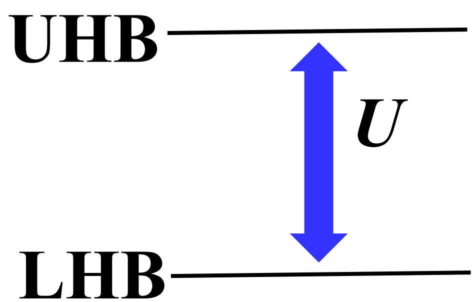
Imada, Suzuki, JPSJ 88, 024701 (2019)

diagonalization of H

$$H=\sum_\sigma[\mu_{\tilde c}\tilde c_\sigma^\dagger\tilde c_\sigma+\mu_{\tilde d}\tilde d_\sigma^\dagger\tilde d_\sigma+\Lambda(\tilde c_\sigma^\dagger\tilde d_\sigma+h.c)],\ \mu_{\tilde c}=\mu_{\tilde d}=-\Lambda=\frac{U}{2}$$

$$\Rightarrow\ \frac{1}{2}(\tilde c_\sigma^\dagger-\tilde d_\sigma^\dagger)=c_\sigma^\dagger n_{-\sigma}$$

$$\frac{1}{2}(\tilde c_\sigma^\dagger+\tilde d_\sigma^\dagger)=c_\sigma^\dagger(1-n_{-\sigma})$$



UHB antibonding of $\tilde c_\sigma$ and $\tilde d_\sigma$

LHB bonding

$$\tilde b_\sigma^\dagger=(\tilde c_\sigma^\dagger+\tilde d_\sigma^\dagger)/\sqrt{2},\ \tilde a_\sigma^\dagger=(\tilde c_\sigma^\dagger-\tilde d_\sigma^\dagger)/\sqrt{2}$$

$$H=\sum_\sigma[E_{\tilde b}\tilde b_\sigma^\dagger\tilde b_\sigma+E_{\tilde a}\tilde a_\sigma^\dagger\tilde a_\sigma],\ E_{\tilde b}=0,E_{\tilde a}=U$$

electron "fractionalization"

UHB ↓ LHB ↓

$$c_\sigma=c_\sigma(n_{-\sigma}+(1-n_{-\sigma}))$$

Mott gap is a "hybridization gap"

gap (mass) generation without SSB

c.f. **CO, AF, Nambu-Jona Lasinio mechanism**

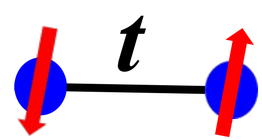
This mapping also works for nonzero *t*

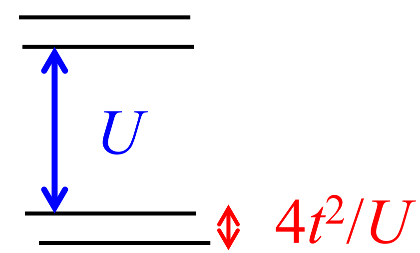
2 sites

$$t_{\tilde c}=t,\ t_{\tilde d}=-t$$

$$E_0=\frac{U}{2}Q, E_1=0, E_2=U,\ E_3=\frac{U}{2}P$$

$$P=1+\sqrt{1+R^2},\ Q=1-\sqrt{1+R^2},\ R=4t/U$$





Correct Mott gap U and superexchange energy $4t^2/U$

Underlying Concept of Fractionalization

Strong coupling superconductivity and quantum spin liquid に見られる共通の機構

強い局所斥力が電荷ギャップを生む(Mottness)
⇔ 2成分への分数化と成分間の混成が創発
自発的対称性の破れを伴わないギャップ（質量）形成

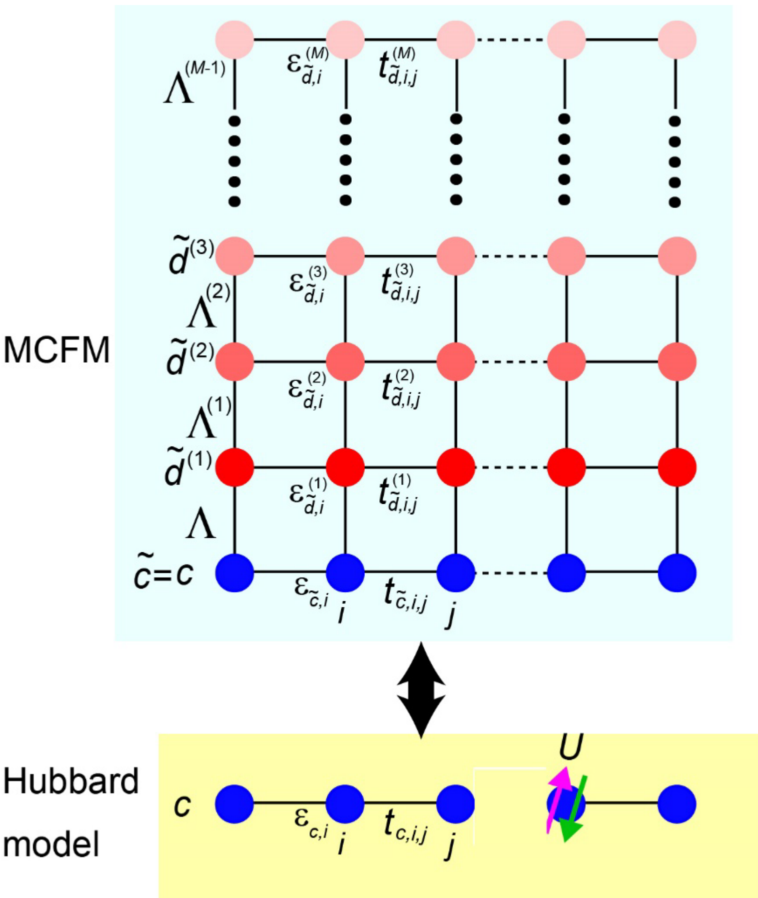
分数化と連動した創発局所引力の発生
(attraction by repulsion)
⇒ 強結合超伝導のクーパー対の起源
⇒ 量子スピン液体のスピン分数化の起源

Fermi machineのアルゴリズムと性質

Neural network algorithm based on fractionalization

$$H = \sum_k [\mu_{\tilde{c}}(k)\tilde{c}_{k\sigma}^{\dagger}\tilde{c}_{k\sigma} + \Lambda_k(\tilde{c}_{k\sigma}^{\dagger}\tilde{d}^{(1)}_{k\sigma} + \mathrm{H.c.}) + \sum_m [\mu_{\tilde{d}}^{(m)}(k)\tilde{d}^{(m)\dagger}_{k\sigma}\tilde{d}^{(m)}_{k\sigma} + \Lambda_k(\tilde{d}^{(m)\dagger}_{k\sigma}\tilde{d}^{(m+1)}_{k\sigma} + \mathrm{H.c.})]$$

MCFM (multi-component fermion model)



$$H = \sum_{k\sigma}\mu_c(k)c_{k\sigma}^{\dagger}c_{k\sigma} + U\sum_i n_{i,\sigma}n_{i,-\sigma}$$

Hubbard

novel neural network/machine learning algorithm

Correspondence between interacting fermions and noninteracting MCFM

RBM; イジング相互作用
FM; もつれを生む、混成

M. IMADA

Procedure of Fermi machine

1. For given MCFM parameters, calculate the ground state w.f. of the MCFM $\left|\Psi_0^{\mathrm{MCFM}}\right\rangle$

2. Map $\left|\Psi_0^{\mathrm{MCFM}}\right\rangle$ to the w.f. of the Hubbard $\left|\Psi_0^{\mathrm{Hub}}\right\rangle$ by the mapping rule

$$\tilde{d}^{(m)}{}_{\ell\sigma} \doteq \tilde{d}^{(m-1)}{}_{\ell\sigma}(1-2n_{\tilde{d}^{(m-1)}{}_{\ell,-\sigma}}), \quad .....$$

$$\tilde{d}^{(1)}{}_{\ell\sigma} \doteq c_{\ell\sigma}(1-2n_{c_{\ell,-\sigma}})$$

$$\left|\Psi_{0\sigma}{}^{\mathrm{Hub}}\right\rangle = \prod_q^{k_F}\left[\sum_{m=0}^{M}\alpha_{m,q}\sum_\ell \frac{e^{iq\ell}}{\sqrt{N_s}}c^\dagger_{\ell,\sigma}(1-2n_{\ell,-\sigma})^m\right]\left|0\right\rangle$$

3. Calculate $\left\langle x \middle| \Psi_0^{\mathrm{Hub}}\right\rangle$ for a given MC sample

4. Perform MC sampling of $\left\langle x\right|$ and calculate $\left\langle E_0\right\rangle = \dfrac{\left\langle \Psi_0^{\mathrm{Hub}}\middle| H \middle|\Psi_0^{\mathrm{Hub}}\right\rangle}{\left\langle \Psi_0^{\mathrm{Hub}} \middle| \Psi_0^{\mathrm{Hub}}\right\rangle}$

$$\Rightarrow \left\langle E_0\right\rangle = \frac{\sum_x \left\langle \Psi_0^{\mathrm{Hub}}\middle| H \middle| x\right\rangle\left\langle x \middle|\Psi_0^{\mathrm{Hub}}\right\rangle^{-1}}{N_{\mathrm{sample}}}, \quad W(x) = \left|\left\langle x \middle| \Psi_0^{\mathrm{Hub}}\right\rangle\right|^2$$

Monte Carlo estimate

5. Optimize the MCFM parameters to lower $\left\langle E_0\right\rangle$

Benchmarks

atomic limit

2 sites

$$\mu_{\tilde{c}} = \mu_{\tilde{d}} = -\Lambda = \frac{U}{2}$$

$$t_{\tilde{c}} = t, \; t_{\tilde{d}} = -t$$

4 sites

half filling

	exact E_0	E_0 by Fermi machine	$t_{\tilde{d}}$	Λ	$\mu_{\tilde{c}}$	$\mu_{\tilde{d}}$
$U=4$	-2.10275	-2.10275	1.0	-1.002	1.002	4.644
$U=8$	-1.32023	-1.32023	1.0	-2.238	2.238	7.229
	-1.32023	-1.32023	2.0	-3.330	3.330	10.731

Exact mapping

hole doped

	exact E_0	E_0 by Fermi machine	Λ	$\mu_{\tilde{c}}$	$\mu_{\tilde{d}}$	$\lambda^{(M)}_{\uparrow,\uparrow} = \lambda^{(M)}_{\uparrow,\uparrow}$	$\lambda^{(M)}_{\uparrow,\downarrow} = \lambda^{(M)}_{\downarrow,\uparrow}$
$U=8$	-3.20775	-3.20775	-2.71408	2.71408	4.73336	-0.35912	-0.71824

$$\Lambda_{\sigma\sigma'}^{(M)}[k] = \lambda_{\sigma\sigma'}^{(M)} \cos[k]$$

Relation to Self-Energy Expansion

Nakajima (1958) – Zwanzig – Mori(1965)

Roth (1969), Mancini, Matsumoto (1996)

Onoda,Imada (2001,2003)

projection operator method

equation of motion method

$$\hat{\omega}A = [A, H]$$

$$\mathcal{P}_1 X = \frac{\langle [X, A^\dagger]_+ \rangle}{\langle [A, A^\dagger]_+ \rangle} A$$

$$i\frac{d}{dt}A(t) \equiv \hat{\omega}A = \mathcal{P}_1\hat{\omega}A + (1-\mathcal{P}_1)\hat{\omega}A$$

$$= \tilde{\varepsilon}^{(11)}A + \delta\hat{\omega}A$$

$$i\frac{d}{dt}\delta\hat{\omega}A(t) = \tilde{\varepsilon}^{(21)}A + \tilde{\varepsilon}^{(22)}\delta\hat{\omega}A + \delta\hat{\omega}\delta\hat{\omega}A$$

$$i\frac{d}{dt}\delta\hat{\omega}\delta\hat{\omega}A(t) = \tilde{\varepsilon}^{(31)}A + \tilde{\varepsilon}^{(32)}\delta\hat{\omega}A + \tilde{\varepsilon}^{(33)}\delta\hat{\omega}\delta\hat{\omega}A + \ldots\ldots$$

$$i\frac{d}{dt}G(t) = \varepsilon^{(11)}G + \delta\hat{\omega}G$$

$$G(\omega) = \frac{1}{\omega - \varepsilon^{(11)} - \Sigma_1(\omega)}$$

$$\Sigma_1(\omega) = \frac{\varepsilon^{(21)}}{\omega - \varepsilon^{(22)} - \Sigma_2(\omega)}$$

....

Continued fraction expansion

Heierarchy in TCFM and MCFM

$$H = \sum_k [\varepsilon_c(k) c_k^\dagger c_k + \Lambda(k)(c_k^\dagger d_k + h.c) + \varepsilon_d(k) d_k^\dagger d_k]$$

$$G = (\omega - H)^{-1} = \begin{pmatrix} \omega - \varepsilon_c & -\nu \\ -\nu & \omega - \varepsilon_d \end{pmatrix}^{-1} = \frac{1}{(\omega-\varepsilon_c)(\omega-\varepsilon_d)-\nu^2} \begin{pmatrix} \omega - \varepsilon_d & \nu \\ \nu & \omega - \varepsilon_c \end{pmatrix}$$

$$G_{cc} = \frac{\omega - \varepsilon_d}{(\omega-\varepsilon_c)(\omega-\varepsilon_d)-\Lambda^2} = \frac{1}{(\omega-\varepsilon_c) - \dfrac{\Lambda^2}{\omega-\varepsilon_d}}$$

$$G = \frac{1}{\omega - \varepsilon_c - \Sigma_1} \qquad \Sigma_1 = \frac{\Lambda^2}{\omega - \varepsilon_d} \to \frac{\Lambda^2}{\omega - \varepsilon_d - \Sigma_2}$$

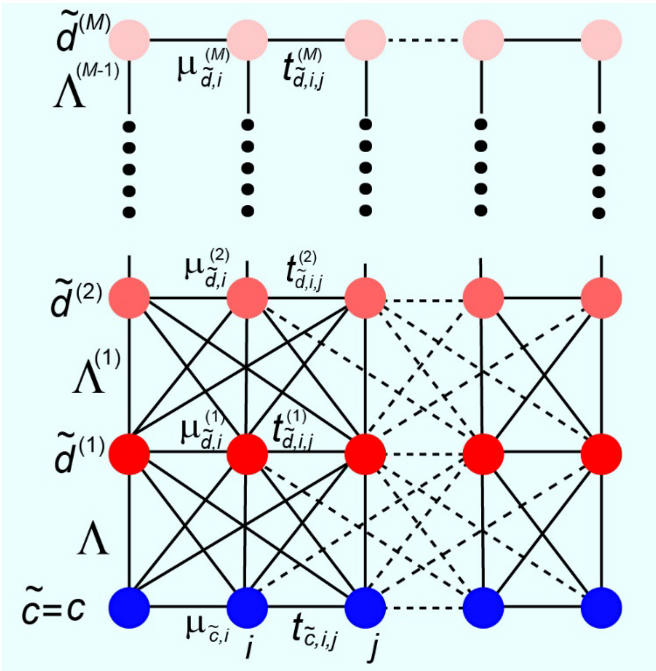
MCFM

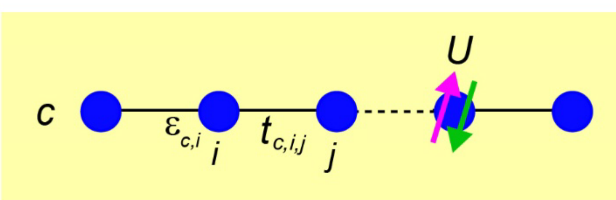
射影演算子法（EOM)の連分数展開と同型

Sakai *et al*. (2016)

Extension to nonlocal coupling

multi-component noninteracting system





Interacting system

$$\tilde{d}^{(m)}{}_{\ell\sigma} \doteq \tilde{d}^{(m-1)}{}_{\ell\sigma}(1-2n_{\tilde{d}^{(m-1)}{}_{\ell,-\sigma}}), \quad .....$$

$$\tilde{d}_{\ell\sigma}^{(m)\dagger} \to \sum_{\ell'\sigma'} \frac{e^{iq(\ell'-\ell)}}{\sqrt{N_S}} \Theta_{\sigma',\sigma}^{(m)}(\ell'-\ell)\tilde{d}_{\ell\sigma}^{(m-1)\dagger}(-)^{n_{\tilde{d}^{(m-1)},\ell',\sigma'}}$$

$$\to \Xi_\sigma^{(m)}(q,\ell)c_{\ell\sigma}^\dagger$$

$$\Xi_\sigma^{(m)}(q,\ell) = \prod_{n=1}^{m}[\sum_{\ell_n,\sigma_n} \frac{e^{iq(\ell_n-\ell)}}{\sqrt{N_S}} \Theta_{\sigma_n,\sigma}^{(m-n+1)}(q,\ell_n-\ell)(-)^{mn_{\ell_n,\sigma_n}}],$$

$$\Xi_\sigma^{(0)}(q,\ell) = 1$$

$$\left|\Psi_{0\sigma}^{\mathrm{Hub}}\right\rangle = \prod_q^{k_F}\left[\sum_{m=0}^{M}\alpha_{mq}\sum_\ell \Xi_\sigma^{(m)}(q,\ell)c_{\ell\sigma}^\dagger\right]|0\rangle$$

Enhance the entanglement of distant electrons

運動方程式の方法(射影演算子やグラムシュミット法）ではなく、非局所カップリングによる一般のNNと同じ戦略でrepresentabilityを高める。

Physical Insight of Mapping

$$\tilde{c}_{\sigma} \doteq c_{\sigma}$$

$$\tilde{d}_{\sigma} \doteq c_{\sigma}(1-2n_{c-\sigma})$$

$$\tilde{d}^{(m)}_{i\sigma} \doteq \tilde{d}^{(m-1)}_{i\sigma}(1-2n_{\tilde{d}^{(m-1)}\ i,-\sigma})$$

Scattering and suppression of double occupation

$$\tilde{d}^{(m)\dagger}_{\ell\sigma} \to \sum_{\ell'\sigma'} \frac{e^{iq(\ell'-\ell)}}{\sqrt{N_S}} \Theta^{(m)}_{\sigma',\sigma}(\ell'-\ell)\tilde{d}^{(m-1)\dagger}_{\ell\sigma}(-)^{n_{\tilde{d}^{(m-1)},\ell',\sigma'}}$$

incorporate nonlocal correlation and entanglement between electrons at (ℓ,σ) and (ℓ',σ')

⇔ nonlocal coupling in RBM, DBM
Jastrow factor in conventional VMC

Optimization of variational parameters α_k

Amari, Neural Comput. 10, 251 (1998).
Sorella PRB 64, (2001) 024512
Tahara, MI JPSJ 77 (2008) 114701

Natural gradient (Stochastic reconfiguration) method

$$\left|\overline{\psi_\alpha}\right\rangle = \frac{1}{\sqrt{\langle \psi_{\bar{\alpha}} | \psi_\alpha \rangle}} \left|\psi_\alpha\right\rangle$$

Consider $\alpha \to \alpha + \gamma$

$$\left|\overline{\psi_{\alpha+\gamma}}\right\rangle = \left|\overline{\psi_\alpha}\right\rangle + \sum_{k=1}^{p} \gamma_k \left|\overline{\psi_{k\alpha}}\right\rangle + O(\gamma^2)$$

$$\left|\overline{\psi_{k\alpha}}\right\rangle \doteq \frac{\partial}{\partial \alpha_k}\left|\overline{\psi_\alpha}\right\rangle = \frac{1}{\sqrt{\langle \psi_\alpha | \psi_\alpha \rangle}} \left(\frac{\partial}{\partial \alpha_k}\left|\psi_\alpha\right\rangle - \frac{\langle \psi_\alpha | \left(\frac{\partial}{\partial \alpha_k}\right) | \psi_\alpha \rangle}{\langle \psi_\alpha | \psi_\alpha \rangle} \left|\psi_\alpha\right\rangle \right)$$

If $\gamma_k = -\Delta t g_k, \quad g_k = \dfrac{\partial E}{\partial \alpha_k}$

$\Rightarrow$ **steepest descent method**

If $\gamma_k = -\Delta t \sum_{l=1}^{p} (h^{-1})_{kl} g_l,$

$h_{kl} = \dfrac{\partial^2 E}{\partial \overline{\alpha_k} \partial \alpha_l}$ $\Rightarrow$ **Newton method**

$$\Delta_{\text{norm}}{}^2 \equiv \left\| \left|\overline{\psi_{\alpha+\gamma}}\right\rangle - e^{-\Delta\tau H}\left|\overline{\psi_\alpha}\right\rangle \right\|^2 \approx \left\| \left|\overline{\psi_{\alpha+\gamma}}\right\rangle - (1-\Delta\tau H)\left|\overline{\psi_\alpha}\right\rangle \right\|^2$$

虚時間発展 $e^{-\tau H}\left|\overline{\psi_\alpha}\right\rangle$
で基底状態へ漸近

$$= \Delta\tau^2 \left\langle \overline{\psi_{\bar{\alpha}}} \right| H^2 \left| \overline{\psi_\alpha} \right\rangle + 2\Delta\tau \gamma_k g_l + \sum_{k,l=1}^{p} \gamma_k \gamma_l S_{kl}$$

$$S_{kl} = \frac{\partial^2}{\partial \overline{\alpha_k} \partial \alpha_l} \left\langle \overline{\psi_{\bar{\alpha}}} \middle| \overline{\psi_\alpha} \right\rangle, \quad g_l = \frac{\partial E}{\partial \alpha_l}, \quad E = \left\langle \overline{\psi_{\bar{\alpha}}} \right| H \left| \overline{\psi_\alpha} \right\rangle$$

variation of
the wave function

$$\gamma_k = -\Delta\tau \sum_{l=1}^{p} S_{kl}{}^{-1} g_l$$

S^{-1}: **stabilize against singular change of the wavefunction**

Optimization of variational parameters α

${}^{T}A$: transpose of A

$$\left|\Psi_{0\sigma}^{\text{Hub}}\right\rangle = \prod_{q}^{k_F}\left[\sum_{m=0}^{M}\alpha_{mq}\sum_{\ell}\Xi_{\sigma}^{(m)}(q,\ell)c_{\ell\sigma}^{\dagger}\right]\left|0\right\rangle$$

1次摂動の表式 $\delta\left|\Psi_0{}^{\text{MCFM}}\right\rangle = \sum_{n\neq 0}\frac{\left\langle\Psi_n{}^{\text{MCFM}}\middle|\delta H_{\text{MCFM}}\middle|\Psi_0{}^{\text{MCFM}}\right\rangle}{E_n - E_0}\left|\Psi_n{}^{\text{MCFM}}\right\rangle$

を使えばH_{MCFM}の変分パラメタを微小量変えた時の波動関数の変化が陽に計算できる。

一方、ハミルトニアンを対角化するユニタリ変換U_αの微小な変化量δU_αが
自然勾配法から求められれば

$$H_{\text{MCFM}} = U_\alpha D_{\text{MCFM}}(U_\alpha)^{-1},\quad \delta U = U_{\alpha+\gamma} - U_\alpha,\quad \delta(U_\alpha{}^{-1}) = \delta({}^{T}U_\alpha) = {}^{T}(\delta U)$$

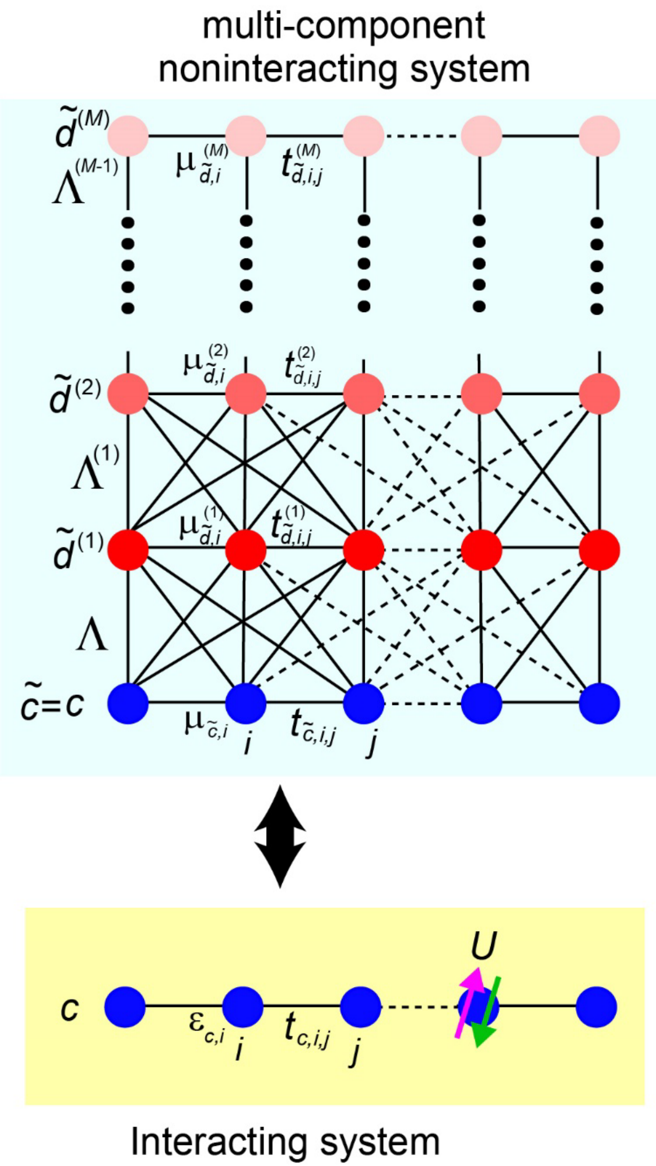
$$\delta H_{\text{MCFM}} = H_{\text{MCFM}}(\xi+\delta) - H_{\text{MCFM}}(\xi) = (\delta U)D^{T}U + UD(\delta^{T}U)$$

より、H_{MCFM}の変分パラメタの変化量がわかる。

H_{MCFM}を対角化する
ユニタリ変換

$$U_\alpha = \begin{pmatrix} \alpha_{m=0,q=q_0}, \alpha_{m=0,q=q_1}, \alpha_{m=0,q=q_2}, \cdots\cdot \\ \alpha_{m=1,q=q_0}, \alpha_{m=1,q=q_1}, \cdots\cdots\cdot \\ \cdots\cdots\cdots \end{pmatrix}$$

Representability



$$\mu^{(m)}_{\tilde{d},i} \to \infty \text{ for odd } m$$

偶数番目の層がすべて孤立

$$H = \sum_k [\mu_{\tilde{c}}(k)\tilde{c}_{k\sigma}^\dagger \tilde{c}_{k\sigma}] + \sum_n [\mu_{\tilde{d}}^{(n)}(k)\tilde{d}^{(n)\dagger}_{k\sigma}\tilde{d}^{(n)}_{k\sigma}]$$

$n=2m$

1. 偶数番目の各層のエネルギーが縮退するように各層のchemical potentialを選べば基底状態は各層の基底状態の任意の線形結合となる.

2. 任意の多体状態は1体状態の直積の線形結合で表せる.
(1体状態の直積は多体状態の完全直交基底を張っている)

$$\left|\Psi^{\mathrm{MCFM}}_{0\sigma}\right\rangle = \sum_{n=1}^{M/2} \alpha_n \prod_q^{k_F} \left|\Psi^{\mathrm{MCFM}}_{\sigma n}(q)\right\rangle$$

$$\left|\Psi^{\mathrm{MCFM}}_{\sigma n}(q)\right\rangle = \tilde{d}^{(n)\dagger}_{q\sigma}\left|0\right\rangle$$

十分大きな*M*を取れば、MCFMの基底状態はHubbard（相互作用系）の多体基底状態を厳密に表わせる。（変分状態）

Discussions and Outlook

J. Phys. Soc. Jpn. 93, 104002 (2024)

Materialization of fractionalization by fermi machine

Interacting fermions

⟷ **Non-interacting multi-component fermions**

cf. holographic correspondence in AdS-CFT,
hidden fermion ⇔ bath in DMFT, DMET
bulk-edge correspondence in topological matter
path int. d dim quantum ⇔ d+1 dim. classical

フェルミマシンの特長、優位性

★ ボルツマンマシンでイジング自由度を使って量子性を取り込むより効率的。

★ VMCで用いる波動関数で対称性を破らずにギャップ構造やグリーン関数のゼロを表わすのは厄介だが、フェルミマシンでは容易。

Outlook

★Efficient optimization of MCFM variational parameters→large systems

★ 隠れ層のホワイトボックス化; 強相関電子系の電子構造が隠れ量子変数の挙動からあぶりだされる可能性

★Better neural network by mapping to HFB (geminal) states by Pfaffian instead of SD?

★Extension to non-periodic such as random systems

Thank you