KEK連携コロキウム・研究会エディション 「量子多体系の素核・物性クロスオーバー」2019.1.14-16 高エネ研つくばキャンパス・4号館セミナーホール

# 高精度量子多体数値計算と機械学習が描き出す ギャップ/質量形成、高温超伝導と暗黒フェルミ粒子

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- 1. Introduction to a grand challenge in condensed matter physics; high  $T_c$
- 2. Progress in numerical methods
- **3. Rejuvenated understanding of cuprate superconductors**
- 4. How does a gap/mass emerge in physics? Cases of condensed matter and particle physics insulating gap, pseudogap and superconducting gap
- 5. How does strong-coupling superconductivity emerge? Dark fermion theory and machine learning
- 6. Summary and outlook

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## Introduction: single-particle Green's function and self-energy Nambu representation for superconductors

$$G = (\omega - H)^{-1} = \begin{pmatrix} \omega - \varepsilon_{\mathbf{k}} - \Sigma^{\text{nor}} & -\Sigma^{\text{ano}} \\ -\Sigma^{\text{ano}} & \omega + \varepsilon_{\mathbf{k}} + \Sigma^{\text{nor}} \end{pmatrix}^{-1} = \begin{pmatrix} G_{11}^{\text{nor}} & F \\ F^* & G_{22}^{\text{nor}} \end{pmatrix}$$

$$G_{11}^{\text{nor}}(\mathbf{k}, \omega) = \begin{bmatrix} \omega + \mu - \varepsilon_{\mathbf{k}} - \left( \Sigma^{\text{nor}}(\mathbf{k}, \omega) + W(\mathbf{k}, \omega) \right) \end{bmatrix}^{-1}$$

$$W(\mathbf{k}, \omega) = \begin{bmatrix} \omega + \mu - \varepsilon_{\mathbf{k}} - \left( \Sigma^{\text{nor}}(\mathbf{k}, \omega) + W(\mathbf{k}, \omega) \right) \end{bmatrix}^{-1}$$

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$$\begin{cases} \langle cc \rangle = \text{Im } F & \mathbf{k} \mathbf{F} \mathbf{r}^{n} \mathbf{F} \mathbf{F}^{n} \mathbf{F}^{n}$$

## Why is $\Sigma^{ano}$ peak important?: How did the BCS el-ph mechanism become convincing?



## How about high $T_c$ cuprate superconductors?



IVL, IVADA

# **One more puzzle; pseudogap**

spin excitation NMR  $T_1$  Yasuoka *et al.* (1989) Knight shift Takigawa et al. (1991) susceptibility Johnston, Nakano et al. MI 🖌 neutron Rossat-Mignod et al.

FL

optical conductivity specific heat Loram et al. μSR

resistivity, Hall coefficient

Raman

. . . . . . . . . .

photoemission, ARPES Shen et al. **STM** 

tunnel conductance

Mott gap beyond AF gap strange metal  $\rho \sim T$ 



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optimization of 1,000-100,000 variables to overcome bias

**Represent strong entanglement in the real space representation** 

IVI, TIVIADA



## **Efficiency and accuracy of TN+VMC**



Zhao *et al.* PRB 96, 085103 (2017)

accuracy beyond each single method

*cf.* Chou *et al.*(2012) Sikora *et al.* (2015)

#### IVI. TIVIA DA



 $\sigma$ ; physical variable

Carleo, Nomura, Imada Nat. Commun. (2018)

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#### VMC+FTTN+LCZS for *ab initio* Hamiltonian of HgBa<sub>2</sub>CuO<sub>4</sub>

Mott gap ~2eV<sub>La based</sub> AF moment ~0.6μ<sub>B</sub> Ohgoe, Hirayama, Ido, Misawa, Yamaji, Imada,

#### Uniform SC state is stabilized for ab intio case

further neighbor transfer and interaction make stripe energy higher

experiments: 0.09<δ<0.12, q~0.25 W. Tabis, Y. Li, M. L. Tacon, et al., Nat. Commun. 5, 5875 (2014). G. Campi, A. Bianconi, et al. S. M. Kazakov, et al., Nature 525, 359 (2015).  $V_3$  partially cancels  $V_1$ 

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# **Origin of gap (mass) generation Spontaneous-symmetry-breaking gap** $c_{k,\sigma}^{\dagger}c_{k+q,\sigma}d_{p,\sigma'}^{\dagger}d_{p-q,\sigma'} \Rightarrow \langle d_{p\sigma'}^{\dagger}c_{p\sigma} \rangle c_{k\sigma}^{\dagger}d_{k\sigma'}$ emergent hybridization $H = \sum \left[ \varepsilon_{c}(k) c_{k\sigma}^{\dagger} c_{k\sigma} + \varepsilon_{d}(k) d_{k\sigma'}^{\dagger} d_{k\sigma'} - \Lambda(k) (c_{k\sigma}^{\dagger} d_{k\sigma'} + h.c) \right]$ <sup>*k* \sigma \sigma'</sup> AF, CO: $d_{k,\sigma} = c_{k+Q,\sigma}$ , SC: $d_{k,\sigma} = c_{-k,-\sigma}^{\dagger}$ $c_{k,\sigma}^{\dagger} c_{k+q,\sigma} (b_{a} + b_{-a}^{\dagger})$ hybridization gap of two-component fermions $\Rightarrow c^{\dagger}_{k,\sigma}c_{k+q,\sigma}c^{\dagger}_{p,-\sigma}c_{p-q,-\sigma}$ $G(\omega) = (\omega - H)^{-1} = \begin{pmatrix} \omega - \varepsilon_c & -\Lambda \\ -\Lambda & \omega - \varepsilon_d \end{pmatrix}^{-1} = \frac{1}{(\omega - \varepsilon_c)(\omega - \varepsilon_d) - \Lambda^2} \begin{pmatrix} \omega - \varepsilon_d & \Lambda \\ \Lambda & \omega - \varepsilon_c \end{pmatrix}$ $G_{c} = \frac{\omega - \varepsilon_{d}}{(\omega - \varepsilon_{c})(\omega - \varepsilon_{d}) - \Lambda^{2}} = \frac{1}{(\omega - \varepsilon_{c}) - \frac{\Lambda^{2}}{\omega - \varepsilon_{d}}} \longrightarrow G_{c}^{\text{bare}} = \frac{1}{\omega - \varepsilon_{c}}$ $\Sigma_{c}^{\text{nor}}(k, \omega) = \frac{\Lambda_{k}^{2}}{\omega - \varepsilon_{d}} \text{ pole of } G_{d}^{\text{bare}} \Leftrightarrow \text{ pole of } \Sigma_{c}^{\text{nor}} \Leftrightarrow \text{ zero of } G_{c}$ if $\varepsilon_d = -\varepsilon_c \Rightarrow \omega = \sqrt{\varepsilon_c (k)^2 + \Lambda_k^2}$ mass generation

**Origin of gap (mass) generation** Nambu-Jona Lasinio **Case of QCD** strong interaction mechanism PR 122, 345 (1961)  $L = \overline{q}(x)(i\gamma^{\mu}D_{\mu} - M)q(x) - \frac{1}{2}\operatorname{Tr}\left[G_{\mu\nu}(x)G^{\mu\nu}(x)\right]$  $q(x) = \begin{pmatrix} u \\ d \\ s \end{pmatrix}, \quad M = \begin{pmatrix} m_u, 0, 0 \\ 0, m_d, 0 \\ 0, 0, m_s \end{pmatrix}, \quad D_\mu = \partial_\mu - ig_s G_\mu T,$ quark interaction through gluon G  $c^{\dagger}d\left(b+b^{\dagger}\right) \Longrightarrow c^{\dagger}\bar{d}c^{\dagger}d$ ator  $c'd(b+b') \Rightarrow c'ac'a$  **quark mass**  $\Rightarrow$  chiral symmetry breaking T;SU(3) generator  $\left\langle \overline{q}_{L}(x)q_{R}(x)\right\rangle \neq 0$ gluon condensation; nonperturbative effect quark-antiquark condensate  $c^{\dagger}d\left(b+b^{\dagger}\right) \Longrightarrow c^{\dagger}d\left(\left\langle b\right\rangle + \left\langle b^{\dagger}\right\rangle\right)$ vacuum condensation similar for weak interaction All require SSB. W-, Z-boson condensation How about the pseudogap **Higgs mechanism** and Mott gap if SSB is absent?



*A*, a constant -*U*/8, has *nothing to do* with the symmetry breaking contrast to AF; Slater mechanism  $f_{k,\sigma} \equiv c_{k+Q,\sigma}, \ \Lambda = U \left\langle c_{k,\sigma}^{\dagger} c_{k+Q,\sigma} \right\rangle$ 

## **Composite fermion for Mott gap**

c, f: fermion operator,

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

exact fermion anticommutation of c and f

$$[c_1, f^{\dagger}]_{+} = 0, \ [f, f^{\dagger}]_{+} = 1, \dots,$$

**diagonalization of** 
$$H = \sum_{\sigma} [\varepsilon_c c_{\sigma}^{\dagger} c_{\sigma} + \varepsilon_f f_{\sigma}^{\dagger} f_{\sigma} + \Lambda(c_{\sigma}^{\dagger} f_{\sigma} + h.c)], \varepsilon_c = \varepsilon_f = \Lambda = -\frac{U}{8}$$

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

$$UHB \qquad UHB \qquad of c and f$$

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

$$UHB \qquad UHB \qquad bonding$$
electron "fractionalization"
$$c_{\sigma} = c_{\sigma}(n_{-\sigma} + (1 - n_{-\sigma}))$$

$$UHB \qquad UHB$$

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## Mott gap and pseudogap, itinerancy and carrier doping



## **Smoking gun for the hidden fermion**

#### **Two-component fermion model at** $T < T_c$

$$H = \sum_{k} [\varepsilon_{c}(k)c_{k\sigma}^{\dagger}c_{k\sigma} + \Lambda_{k}(c_{k\sigma}^{\dagger}d_{k\sigma} + \text{H.c.}) + \varepsilon_{d}(k)d_{k\sigma}^{\dagger}d_{k\sigma}$$

$$+(\Delta_{c}c_{k\sigma}^{\dagger}c_{k\sigma}^{\dagger} + \Delta_{d}d_{k\sigma}^{\dagger}d_{k\sigma}^{\dagger} + \text{H.c.})] \text{Nambu representation}$$

$$\Sigma_{c}^{\text{nor}}(k,\omega) = G_{d}\Lambda_{k}^{2} = \frac{\Lambda_{k}^{2}}{(\omega - \varepsilon_{d}) - \frac{\Delta_{d}^{2}}{\omega + \varepsilon_{d}}} \text{Act matrix}$$

$$\Sigma_{c}^{\text{ano}}(k,\omega) = \Delta_{c} + G_{d}\Lambda_{k}^{2} = \Delta_{c} + \frac{\Lambda_{k}^{2}\Delta_{d}(\omega + \varepsilon_{d})}{(\omega - \varepsilon_{d}) - \frac{\Delta_{d}^{2}}{(\omega + \varepsilon_{d})}}$$

$$G(\mathbf{k},\omega) = \left[\omega + \mu - \varepsilon_{\mathbf{k}} - \Sigma_{c}^{\text{nor}}(\mathbf{k},\omega) - W(\mathbf{k},\omega)\right]^{-1} \text{The poles cancel in }\Sigma^{\text{nor}} + W$$

$$W(\mathbf{k},\omega) = \frac{\Sigma_{c}^{\text{ano}}(\mathbf{k},\omega)^{2}}{\omega - \mu + \varepsilon_{\mathbf{k}} + \Sigma_{c}^{\text{nor}}(\mathbf{k},-\omega)^{*}} \text{smoking gun } 0A$$

## Pole cancellation between $\Sigma^{nor}$ and $\Sigma^{ano}$

 $G(\mathbf{k},\omega) = \left[\omega + \mu - \varepsilon_{\mathbf{k}} - \Sigma^{\text{nor}}(\mathbf{k},\omega) - W(\mathbf{k},\omega)\right]^{-1}$ Sakai *et al.* Phys. Rev. Lett.  $W(\mathbf{k},\omega) = \frac{\Sigma^{\text{ano}}(\mathbf{k},\omega)^2}{\omega - \mu + \varepsilon_{\mathbf{k}} + \Sigma^{\text{nor}}(\mathbf{k},-\omega)^*} \quad \Sigma^{\text{nor}} \text{ cancels with } W ! 116 \text{ (2016) 057003}$ **Perfect agreement** 8 T < T<sub>c</sub> with TCFM 4 A(k,ω)×10 Poles of  $\Sigma^{nor/ano}$  are **The reason why** invisible in  $A(\mathbf{k}, \omega)$ . = overlooked in 0 experiments U=8t t'=-0.2t If the peak directly comes from  $\dots$  Im $\Sigma^{nor}$ n=0.95 --- ImW -8 bosonic excitations such as T=0.01  $Im(\Sigma^{nor}+W)$  $k=k_{AN}$ spin fluctuations, -1.5 -1 -0.5 0.5 0  $(\mathbf{0})$ the cancellation does not happen.  $A(\mathbf{k},\omega) = -\frac{1}{-1} \operatorname{Im} G(\mathbf{k},\omega)$ **Evidence for hidden fermion** Why is the peak important? [ADA]



80% of the gap is attributed to the peak! What makes this peak? = What is the hidden fermion?

## $A(k,\omega)$ ; comparison between ARPES data and machine learning



# **Summary**

- 1. VMC, tensor network, neural network as quantum many-body solvers without sign problem
- 2. Severe competition between SC and charge inhomogeneity (PS and stripes)
- 3. *Ab initio* Hamiltonian reproduces the phase diagram of cuprates
- 4. Universal gap (mass) generation by hybridization gap without SSB (Mott gap, pseudogap)
- 5. Prominent self-energy peak generating SC with cancellation ⇒ dark fermion theory
- 6. Machine learning of ARPES supports dark fermion theory and Planckian dissipation



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**Bose condensation, without spontaneous symmetry breaking** 

contrast with el.-photon and el.-phonon coupled system, W, Z bosons and gluons

## **Exciton and hidden fermion**

electron weakly bound to a hole (Wannier type)  $\beta = g_{d\delta} c_{j\sigma}^{\dagger} (1 - \alpha_{\delta} n_{j+\delta,-\sigma}) (1 - \beta_{\delta} n_{j+\delta,\sigma}) \delta = 0$  $d_{j,\delta,\sigma}^{\dagger} = g_{d\delta} c_{j\sigma}^{\dagger} (1 - \alpha_{\delta} n_{j+\delta,-\sigma}) (1 - \beta_{\delta} n_{j+\delta,\sigma}) \delta = 0$ hidden fermion creation  $\alpha_{\delta} \sim 1, \beta_{\delta} \sim 1$  j  $j+\delta$   $d_{j,\delta,\sigma}^{\dagger} = 0$ 



exciton

 $t\sum_{\delta} d^{\dagger}_{j,\delta,\sigma} c_{k\sigma} b_{j,\delta} + \text{H.c.} \implies t\sum_{\delta} d^{\dagger}_{j,\delta,\sigma} c_{k\sigma} \left\langle b_{j,\delta} \right\rangle + \text{H.c.}$  $d^{\dagger} \qquad \text{hybridization gap} \sim t^2/U$ 

Imada, Suzuki, JPSJ (2019) IMA TIMA DA