Overcoming Fermionic Sign Problem in Lattice Quantum Monte Carlo: a Cuprate Case

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### **Outline**

- HTSC: Cuprate case
- Reference system: DF-QMC method
- What is "Glue" for HTSC?

4 havior the rapplicability of Fermi-liquid theory (which e showing super dence of the resistancy observed in the overdoped metallic regime was taken as evidence for *Fermi-liquid be*describes electronic excitations in terms of an interacting regnie was taken as evidence for *reimi-uquid be-*



C. Proust and L.Taillefer, Annu. Rev. Condens. Matter Phys. 10, 409-429 (2019) C. Proust and L.Taillefer, Annu. Rev. Condens. Matter Phys. 10, 409–429 (2019)



FIG. 1. Phase diagram  $s$ h $x$ ing  $s$ uperconduction

pseudogap, and normal-

**Fig. 1.** Temperature dependence of resistivity in Ba<sub>x</sub>La<sub>S</sub>  $\leq$   $\leq$   $\log_5$  (a  $\leq$   $\gamma$ ) for samples with  $x(Ba) = 1$  (upper curves, left scale) and  $x(Ba) = 0.75$  (lower curve, right scale). The first two cases also s influence of current density

*3. Conductivity Measurements*  J. Bednorz and K. Müller Z. Phys. B 64, 189 (1986) method. Rectangular-shaped samples, cut from the



J. Sobota, Yu He, and Zhi-Xun Shen, RMP 93, 025006 (2021)  $\ldots$  exterit, the CuOn− middle inset the CuOn−, copper; gray circle, cop J. Sobota, Yu He, and Zhi-Xun Shen, RMP 93, 025006 (2021)



# Complicated Stripes-HTSC problem

?

"Absence of Superconductivity in the Pure T two-Dimensional Hubbard Model"

S.R. White, S.W. Zhang et al. PRX10, 031016 (2020)

"Coexistence of superconductivity with partially filled stripes in the Hubbard model" S.R. White, S.W. Zhang et al. Science 384, 637 (2024)





### Fermionic QMC: sign problem vs. sign blessing



<sup>6,2</sup> <sup>6,2</sup> <sup>6,2</sup> N. Prokof'ev "DiagMC" Jülich school 2019

### ng: QMC

<sup>2</sup>*U*1234*c*3*c*<sup>4</sup>



JETP Lett. 64, 911 (1996), Sov. Phys. JETP 87, 310 (1998) N. Prokof'ev, B. Svistunov, Phys. Rev. Lett. 81, 2514 (1998)  $CT-QMC: CT-INT ("det G<sub>0</sub>")$  $\sum_{i=1}^n$ integrals and input to Eq. (1). Thus, regardless of the  $\sum_{i=1}^n$ for two propagators the number of loops changes by *±*1 and this leads to an additional factor JEIP LETT. 64, YII (1996), SOV. any property subset of contracting  $C$ , *S* (  $\alpha$   $\alpha$   $\beta$  )  $\beta$  (  $\alpha$   $\beta$  )  $\alpha$  (

A. Rubtsov, and A. L., JETP Lett. 80, 61 (2004)

A. Rubtsov, V. Savkin, and A. L., Phys. Rev. B 72, 035122 )2005)

CDet:  $\Delta t$  $C(V) = \det(V) - \sum C(S) \det(V \setminus S)$  $S{\subsetneq}V$  $C(S) \det(V \backslash S)$ 

R. Rossi, Phys. Rev. Lett. 119, 045701 (2017) particular set of parameters has to be viewed as a point in *{*⌫*}*. Accordingly, the modulus of *D*⌫ R. Rossi, Phys. Rev. Lett. 119, 045/01 (2017)

will need to interact also the configuration "phase," ' $\alpha$  = arg  $D$  (the diagram phase is diagram pha Strong: U>>t complicated perturbation diagram scales as *n*<sup>3</sup> 2*<sup>n</sup>*, where 2*<sup>n</sup>* comes from the combinatorial number of possible proper subsets,

```
2.1 Updates: general principles
CT-QMC: CT-HYB ("det D")
m=1 n!/m!(n  m)!. The number of arithmetic operations required to solve these recursive
```
 $T_{\text{max}}$  processes of  $\frac{1}{2}$  and  $\$ Phys. Rev. Lett. 97, 076405 (2006). P. Werner, A. Comanac, L. de' Medici, M. Troyer, A. Millis improvement compared to the (*n*!)<sup>2</sup> scaling of the total number of connected graphs. After sum-



### Super-perturbation: DF-QMC

- Controllable perturbative solution of doped Hubbard model for HTSC
- Developed DF expansion around DQMC for N=1, t'=0



DQMC – no sign problem DF QMC super-perturbation

# DOS for Reference System





S. Brener, E. Stepanov, A. Rubtsov, M. Katsnelson, A.L., Ann. Phys. 422, 168310 (2020)

Similar "strong-coupling" cumulant expansion:

S.K. Sarker, JPC 21, L667 (1988) S. Pairault et al, EPJ B16, 85 (1990) W. Metzner, PRB 43, 8549 (1991)

#### DF-QMC scheme: Real Space neme: Real Snace including the the chemical potential points in the chemical potential  $\mathcal{L}$ agon i Gr  $\Gamma^4$   $\Omega^4$   $\Omega^4$  super-perturbation  $\Gamma$ fermion expansion around arbitrary reference system within the path-integral formalbomer Dee  $\mathsf{S}\mathsf{H}\mathsf{G}.$  Neal opace heme: Real Space is the two-pace echama: Raal Snaca scheme. Real opace energy equal dual Green's function  $\sim$  $\Gamma^4$   $\Omega^3$  40 are spin-indices. <sup>1234</sup> = h*c*1*c* ⇤ <sup>2</sup>*c*4*c* ⇤ <sup>3</sup>ih*c*1*c* ⇤ <sup>2</sup>ih*c*4*c* ⇤ <sup>3</sup>i + h*c*1*c* The first order for the vertex in particle-hole (PH) channel is given by the diagram of perhamed Deal Green *G*˜0 <sup>12</sup> = h *t* ˜ <sup>1</sup> *<sup>g</sup>*<sup>ˆ</sup> <sup>12</sup> (6)

 $\sqrt{2}$ 

*t* if *i* and *j* are nearest neighbours,

 $\begin{bmatrix} 0 & \text{other Wisc,} \\ \end{bmatrix}$ 

 $\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$ 

*U*1234*c*⇤

 $O_{12} - [8 + 2j - 4]_{12}$ 

 $\mathbb{R}^2$ 

<sup>1</sup> (G↵)

 $\alpha t'$  if *i* and *j* are next nearest neighbours,

 $P_{\text{total}}$  defined a  $\alpha$  = 0, 1, which defined a  $\alpha$ 

 $\overline{1}$ 

 $\mathcal{G} = \mathcal{G}_0^{-1} - \mathcal{G}_1^{-1}$ 

 $\begin{bmatrix} -1 \\ 1 \end{bmatrix}$ 

 $\overline{1}$  ( $\overline{1}$ )

cutted from infinite lattice and then force translation symmetry and periodic boundary

 $u_{ij} = \begin{cases} \alpha \mu & \text{if } i = j, \\ 0 & \text{otherwise,} \end{cases}$ 

 $\left\{\right.$ 

 $\overline{\phantom{a}}$ 

 $\begin{bmatrix} \alpha\mu \\ 0 \end{bmatrix}$ 

 $\left\{ \begin{matrix} 0 & \text{other} \end{matrix} \right\}$ 

12 a

 $\alpha\mu$  if  $i = j$ ,

0 otherwise,

*d d*<sub>1</sub> *d*<sub>1</sub> *d*<sub>1</sub> *d*<sub>1</sub> *d*<sub>1</sub> *d*<sub>1</sub> *d*<sub>1</sub> *d*<sub>1</sub>

 $t_{ij}^{\alpha} = \begin{cases} \alpha t' & \text{if } i \text{ and } j \text{ are next nearest nearly} \end{cases}$ 

 $\left\{ \begin{array}{ll} 0 & \text{otherwise,} \end{array} \right.$ 

*w*ise,

 $\alpha$  therwise.

hamiltonian and A ism [27, 24] similar to a strong coupling expansion [43]. In this case our *N* ⇥ *N*  $\begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 \ 1 & 1 & 1 & 1 & 1 & 1 \ 1 & 1 & 1 & 1 & 1 & 1 \ 1 & 1 & 1 & 1 & 1 & 1 \ 1 & 1 & 1 & 1 & 1 & 1 \ 1 & 1 & 1 & 1 & 1 & 1 \ 1 & 1 & 1 & 1 & 1 & 1 \ 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix}$ Hamiltonian and Action Hamiltonian and Action <u>in</u> and <u>Action 2</u>

$$
\hat{H}_{\alpha} = \sum_{i,j,\sigma} t_{ij}^{\alpha} c_{i\sigma}^{\dagger} c_{j\sigma} + \sum_{i}^{V} U(n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2})
$$
\n
$$
t_{ij}^{\alpha} = \begin{cases}\nt & \text{if } i \text{ and } j \text{ are nearest neighbours,} \\
\alpha t' & \text{if } i \text{ and } j \text{ are next nearest neighbours,} \\
\alpha \mu & \text{if } i = j,\n\end{cases}
$$
\notherwise,

$$
S_{\alpha}[c^*, c] = -\sum_{1,2} c_1^* \left(\mathcal{G}_{\alpha}\right)_{12}^{-1} c_2 + \frac{1}{4} \sum_{1234} U_{1234} c_1^* c_2^* c_4 c_3
$$
 Perturbation:  $\tilde{t} = \mathcal{G}_0^{-1} - \mathcal{G}_1^{-1}$   
Dual Action:

 $S-OMC$  3.4

3,4

 $g_{\mu}$  $g_{\mu}$   $g_{\mu}$ 

*sQMC*

 $\frac{12}{\sqrt{24}}$ 

Dual Action:

Dual Action:

\n
$$
\tilde{S}[d^*,d] = -\sum_{12 \text{ y}\sigma} d^*_{1\text{ y}\sigma} (\tilde{G}^0_{\text{ y}})^{-1}_{12} d_{2\text{ y}\sigma} + \frac{1}{4} \sum_{1234} \gamma_{1234} d^*_{1} d^*_{2} d_{3} d_{4} + \dots
$$
\nDual GF:

\n
$$
\tilde{G}^0_{12} = \left[ \tilde{t}^{-1} - \hat{g} \right]_{12}^{-1}
$$
\nVertex:

\n
$$
\text{g exact GF of H}_0
$$
\n1-st order diagram

\n
$$
\begin{bmatrix}\n\frac{4}{1} & 3 \\
\frac{1}{2} & \frac{2}{5}\n\end{bmatrix}
$$
\nFinal GF:

\n
$$
\tilde{\Sigma}^{(1)}_{12} = -\sum_{r \in \text{OMC}} \sum_{234} \gamma^d_{1234}(s) \tilde{G}^0_{34}
$$
\nFinal GF:

\n
$$
G_{12} = \left[ \left( g + \tilde{\Sigma} \right)^{-1} - \tilde{t} \right]_{12}^{-1}
$$

Inside QMC - Wick:  $\gamma_{1234}(s) \equiv \langle c_1 c_2^* c_3 c_4^* \rangle_s = \langle c_1 c_2^* \rangle_s \langle c_3 c_4^* \rangle_s - \langle c_1 c_4^* \rangle_s \langle c_3 c_2^* \rangle_s$ ism [27, 24] similar to a strong coupling expansion [43]. In this case our *N* ⇥ *N*  $y_{1234}(s) = \frac{c_1 c_2 c_3 c_4}{s} - \frac{c_1 c_2}{s} + c_3 c_3 c_4}{s} - \frac{c_1 c_2}{s}$ QIVIC - WICK. *sQMC* 3,4  $\frac{1}{2}$   $\frac{2}{3}$   $\frac{4}{3}$   $\frac{1}{2}$   $\frac{2}{3}$   $\frac{3}{3}$   $\frac{4}{3}$   $\frac{4}{3}$  $\gamma_{1234}(s) \equiv \langle c_1 c_2^* c_2 c_3^* \rangle_s = \langle c_1 c_2^* \rangle_s \langle c_2 c_4^* \rangle_s - \langle c_1 c_4^* \rangle_s \langle c_2 c_2^* \rangle_s$  $OMC = V$  $\mathbf{v}$  $\lim_{x \to \infty}$  $12$  $\left(\begin{array}{ccc} 1 & 1 \\ 0 & 1 \end{array}\right)$ *d*  $\overline{\phantom{a}}$  $y_{1234}(9) = \frac{16}{26} \frac{26}{36} \frac{4}{s} - \frac{16}{2} \frac{16}{s} \frac{26}{s} \frac{4}{s}$ Inside QMC - Wick:  $\gamma_{1234}(s) \equiv \langle c_1 c_2^* c_3 c_4^* \rangle_s = \langle c_1 c_2^* \rangle_s \langle c_3 c_4^* \rangle_s - \langle c_1 c_4^* \rangle_s \langle c_3 c_2^* \rangle_s$  $s(s) = \langle c, c^*c, c^* \rangle = \langle c, c^* \rangle \langle c, c^* \rangle - \langle c, c^* \rangle \langle c, c^* \rangle$  $\gamma_{1234}(s) \equiv \langle c_1 c_2^* c_3 c_4^* \rangle_s = \langle c_1 c_2^* c_3^* c_4^* \rangle_s$ 

**lattice and corresponding reference systems represent**  $\tilde{\mathcal{B}}_{12}^s$  $\mathcal{L}_{\text{1}}$ inite and periodise the general lattice and g $\mathcal{L}_{\text{2}}$ ubtraction  $g_{12}^s = g_{12}^s - g_{12}$ **g**<sub>12</sub>  $12$  $-812 - 812$ Disconnected part - subtra and the final Green's function reads 10 Disconnected part - subtraction  $\tilde{g}_{12}^s = g_{12}^s - g_{12}$ 

### Super-DF-QMC 2x2 compare with exact QMC



#### DF-QMC scheme: K - Space E-Space with with the dual action in Space For large system (*N* 4) it is much faster to calculate the dual self-energy in the K-space with within the QMC Markov chain. The dual action in K-space reads  $R-F$  and  $\alpha$  in The dual action in The dual action in The dual action in  $K-$ 1 For transformation of the vertex *<sup>d</sup>* X. *kk*<sup>0</sup> *gkkk*<sup>0</sup> (15) <sup>1234</sup> in Eq. (9)within the QMC step in the K-space *<sup>k</sup>* = *<sup>k</sup> g*ˆ*<sup>k</sup>* Bince the bare of the the space in the independent of  $\mathcal{L}$ *ne k* - *Space*

Action in Fourier-space  $\tilde{S}[d^*,d] = \sum$  $\mathbf{k} \nu \sigma$  $d^*_{\mathbf{k}\nu\sigma}$   $\tilde{G}^{-1}_{0\mathbf{k}\nu}$   $d_{\mathbf{k}\nu\sigma}$  + 1 4  $\sum$ 1234  $\gamma_{1234}d_1^{*}d_2^{*}d_3d_4$  $\overline{a}$   $\overline{a}$ **in Fourier-space**  $k \equiv (\mathbf{k}, v_n)$  and  $v_n = (2n + 1)\pi/\beta$ .  $\sum_{x} x^2 + 1$  $V_n = (2n + 1)\pi/\beta$  **k**  $v\sigma$  **d**  $\frac{2\pi}{\beta}$  **d**  $\frac{2}{\beta}$  **2 Z** Action in Fourier-space<br> $\tilde{\sigma}$   $\tilde{\sigma}$   $\tilde{\sigma}$  are  $\tilde{\sigma}$  are  $\tilde{\sigma}$   $\tilde{\sigma}$  are to  $\tilde{\sigma}$  and  $\sigma$  $k = (\mathbf{k}, v_n)$  and  $v_n = (2n+1)\pi/\beta$   $\begin{array}{c} \mathcal{S}[\boldsymbol{u}, \boldsymbol{u}] = -\sum_{\mathbf{k} \gamma \sigma} u_{\mathbf{k} \gamma \sigma} \mathbf{G}_{0\mathbf{k} \gamma} u_{\mathbf{k} \gamma \sigma} + \frac{1}{4} \sum_{1234} \gamma_{1234} u_1 u_2 u_3 u_4 \end{array}$  $\approx 0 \quad (1 \quad \lambda^{-1})$ the reference system, it is fully translationally invariant *G*˜0 Fourier-space  $\tilde{S}[d^*d] = -\sum d^* \quad \tilde{G}^{-1}d \cdot \frac{1}{4} \sum_{\lambda} \chi_{\lambda} \otimes d^*d^*d_{\lambda}d_{\lambda}$  $\sum_{\mathbf{k}\gamma\sigma}$   $\sum_{\mathbf{k}\gamma\sigma}$   $\sum_{\mathbf{k}\gamma\sigma}$   $\sum_{\mathbf{k}\gamma\sigma}$   $\sum_{\mathbf{k}\gamma\sigma}$   $\sum_{\mathbf{k}\gamma\sigma}$   $\sum_{\mathbf{k}\gamma\sigma}$   $\sum_{\mathbf{k}\gamma\sigma}$   $\sum_{\mathbf{k}\gamma\sigma}$   $\sum_{\mathbf{k}\gamma\sigma}$ lationally invariant therefore *g<sup>s</sup>* <sup>12</sup> = h*c*1*c*⇤ <sup>2</sup>i*<sup>s</sup>* and we use double Fourier transform to  $\frac{1}{3}$ where  $\tilde{S}[d^*d] = \sum d^*$  and  $\tilde{C}^{-1}d = \sum d^*d^*d^*d^*d^*d$  $\mathbf{G}_{n} = (2n+1)\pi/\beta$   $\mathbf{G}_{n}$   $\$ indices  $\mathcal{I}^{(2)}$  become translation  $\mathcal{I}^{(2)}$  become translation, which finally leads  $\mathcal{I}^{(2)}$  $I_n - g_{n+1}$  subtractions has the following form  $S[d^*,d]$ *kk*<sup>0</sup> *gkkk*<sup>0</sup> (15)

Bare dual GF: 
$$
\tilde{G}_k^0 = (\tilde{t}_k^{-1} - \hat{g}_k)^{-1}
$$

Fourier transform to calculate the K-space dual Green's function *G*˜0 First order diagram energy ⌃˜ *<sup>k</sup>*

$$
\tilde{\Sigma}_{k}^{(1)} = \frac{-1}{(\beta N)^{2}Z_{QMC}} \sum_{s-QMC} \sum_{k'} \left[ \tilde{g}_{kk}^{\uparrow\uparrow} \tilde{g}_{kk'}^{\uparrow\uparrow} - \tilde{g}_{kk'}^{\uparrow\uparrow} \tilde{g}_{kk'}^{\uparrow\uparrow} + \tilde{g}_{kk}^{\uparrow\uparrow} \tilde{g}_{k'k'}^{\downarrow\downarrow} \right]_{s} \tilde{G}_{k'}^{0}
$$

lation of disconnected part<sup>.</sup> ction of disconnected part:  $\tilde{g}^s_{kk'}=g^s_{kk'}-g_k\delta_{kk'}$ calculate *g<sup>s</sup>*  $\frac{1}{2}$  . The vertex in eq. (7) we just in the vertex in the Subtraction of disconnected part: substract exact Green's function from the previus QMC run of the reference system as (1)2 part:  $g_{kk'} - g_{kk'} - g_{k} v_{kk'}$ *sQMC k*0 *<sup>k</sup>*0*k*<sup>0</sup> *g*˜ *kk*0*g*˜ *<sup>k</sup>*0*<sup>k</sup>* + *g*˜

 $f^{\prime}$ For transformation of the vertex *<sup>d</sup>*  $\mathsf{Lattice}$  calculations introduced over two spin projections.

Lattice Green's function 
$$
G_k = \left[ \left( g_k + \tilde{\Sigma}_k \right)^{-1} - \tilde{t}_k \right]^{-1}
$$

 $N.B.: \tilde{\Sigma}_k = 0$  corresponds to CPT approximation  $N.B.: \Sigma_k = 0$  corresponds to CPT approximation ponds to CPT ap<sub>l</sub> *t* roxi  $\mathbf{u} \in \tilde{\mathbf{u}}$  to the final spin-up components of the first order dual selfenergy **N.B.:**  $P(X, B)$ :  $\tilde{\Sigma}_k = 0$  corresponds to CPT approximation  $N.B.: \tilde{\Sigma}_k =$  *t* ˜ *k* 1<br>1 esponds to CPT approxir

### K-space test 4x4 system DQMC & CT-INT

DF-1 order







 $U/t=2$  $T/t=0.2$ 

DF-2 order







 $\omega$ 



# Spectral Function anti-nodal and node and node of the section of the section of  $\mathcal S$





# DF-QMC for 8x8: Spectral Function



S. Iskakov, et al, npj Computational Materials 10, 36 (2024)

# Nodal-Antinodal dichotomy



#### Superconductivity: D-wave instability tv: D-wave Instabil k,k0,q ⌫,⌫0,! {} k,⌫ <sup>k</sup>,⌫,"; *<sup>f</sup>* k,⌫,# <sup>k</sup>,⌫,"; *<sup>f</sup>* ⇤ k,⌫,# sioonddocivity. D

Perturbation action with external symmetry breaking fields  $\Delta_k = h_{dw}(\cos k_x - \cos k_y)$ Perturbation action with external symmetry bre

$$
\Delta S = \sum_{\mathbf{k},\nu,\sigma} c_{\mathbf{k},\nu,\sigma}^{*} \tilde{t}_{\mathbf{k},\nu} c_{\mathbf{k},\nu,\sigma} + \sum_{\mathbf{k},\nu} \Delta_{\mathbf{k}} \left( c_{\mathbf{k},\nu,\uparrow}^{*} c_{-\mathbf{k},-\nu,\downarrow}^{*} - c_{-\mathbf{k},-\nu,\uparrow} c_{\mathbf{k},\nu,\downarrow} \right)
$$

Bare Dual Green's Function - Spinor From The bare dual Green's function

$$
\tilde{\mathcal{G}}_{\nu} = \begin{bmatrix} \tilde{t}_{\mathbf{k},\nu} & \Delta_{\mathbf{k}} \\ \Delta_{\mathbf{k}} & -\tilde{t}_{-\mathbf{k},-\nu} \end{bmatrix}^{-1} - \begin{bmatrix} g_{\mathbf{k},\nu}^{\uparrow} & 0 \\ 0 & -g_{-\mathbf{k},-\nu}^{\downarrow} \end{bmatrix}^{-1}
$$

Dual Self-energy - Spinor From with the coefficient  $\alpha$  in the coefficient  $\alpha$  in the gets performation standard dual transformations, one gets  $\alpha$ Here, we define the composite index *k* 2 {k 2 }. The composite index *k* 2 {k and the lattice Green's function can be a captive Green's function can be a captive Green's function can be a captive Green's function can be a  $\mu$ using bein-energy with the matrix form: leads us to the following equation for final spin-up components of the final spin-up components of the first order dual spin-up components of the final spin-up components of the final spin-up components of the first order Bual Self-energy – Spinor-From

$$
\tilde{\Sigma}_{k}^{\uparrow\uparrow} = \frac{-1}{Z} \sum_{\mathcal{QMC}} \sum_{k'} \left[ \left( \tilde{g}_{kk}^{\uparrow} \tilde{g}_{k'k'}^{\uparrow} - \tilde{g}_{kk'}^{\uparrow} \tilde{g}_{k'k}^{\uparrow} \right) \tilde{G}_{k'}^{\uparrow\uparrow} + \tilde{g}_{kk}^{\uparrow} \tilde{g}_{k'k'}^{\downarrow} \tilde{G}_{k'}^{\downarrow\downarrow} \right] \qquad \qquad \tilde{\Sigma}_{k}^{\uparrow\downarrow} = \frac{1}{Z} \sum_{\mathcal{QMC}} \sum_{k'} \tilde{g}_{kk'}^{\uparrow} \tilde{g}_{k'k}^{\downarrow} \tilde{G}_{k'}^{\uparrow\downarrow} \n\tilde{\Sigma}_{k}^{\downarrow\downarrow} = \frac{-1}{Z} \sum_{\mathcal{QMC}} \sum_{k'} \left[ \left( \tilde{g}_{kk}^{\downarrow} \tilde{g}_{k'k'}^{\downarrow} - \tilde{g}_{kk'}^{\downarrow} \tilde{g}_{k'k}^{\downarrow} \right) \tilde{G}_{k'}^{\downarrow\downarrow} + \tilde{g}_{kk}^{\downarrow} \tilde{g}_{k'k'}^{\uparrow} \tilde{G}_{k'}^{\uparrow\uparrow} \right] \qquad \qquad \tilde{\Sigma}_{k}^{\downarrow\uparrow} = \frac{1}{Z} \sum_{\mathcal{QMC}} \sum_{k'} \tilde{g}_{kk'}^{\downarrow} \tilde{g}_{k'k}^{\uparrow} \tilde{G}_{k'}^{\downarrow\uparrow}
$$

#### Superconductivity: D-wave instability  $\mathbb{R}^2$ *k*0 **T** D-waye instability

Lattice Green's Function: Spinor Form: For the HTSC-field corresponding Green's function reads

$$
G_k = \begin{bmatrix} \begin{pmatrix} g_k + \tilde{\Sigma}_k^{\uparrow\uparrow} & \tilde{\Sigma}_k^{\uparrow\downarrow} \\ \tilde{\Sigma}_k^{\downarrow\uparrow} & -g_k^* + \tilde{\Sigma}_k^{\downarrow\downarrow} \end{pmatrix}^{-1} - \begin{pmatrix} \tilde{t}_k & 0 \\ 0 & -\tilde{t}_k^* \end{pmatrix} \end{bmatrix}^{-1}
$$



### Fermi Surface and d-waves: Superconductivity of the "bad" electrons

Normal:  $A(k) = -1/\pi G(k,\omega_0)$  Anomalous: F  $(k,\omega_0)$ 



16x16 lattice U=5.6 t'/t=-0.3 T=0.2t

# Effect of t'



Dw(X)/h

# Effect of eVH

8x8-Hubbard Dw-mat at X



#### ED 4x4 cluster: Local Pairs  $\sum_{n=1}^{\infty} 1 \cdot 1$  cluster Lead Deire D 4X4 cluster: Local Pairs ground pairs



M. Danilov, E.G.C.P. van Loon, S. Brener, S. Iskakov, M. Katsnelson, and A.L.<br>npi Quantum Materials **7** 50 (2022) occurs at *t* <sup>152</sup> /*t* ⇡ 0.12). The binding of the two holes becomes extremely strong around npj Quantum Materials **7,** 50 (2022)  $F(0,0,0)$  pseudogap formation in (4  $\mu$ ) periodic cluster from the peak DOS structure of individual 2  $\mu$ **E.G.C.P. van Loon. S. Brener. S. Iskakov. M. Katsnel** M. Danilov, E.G.C.P. van Loon, S. Brener, S. Iskakov, N

#### Strong Coupling HTSC: RVB trong Coupling HTSC: RVB  $C_{trans} \cap C_{11}$ energies on some detail before the some detail before the some that Heisenberg model plus small contributions from doubly OCCCC SITES. IN THE SIGNAL SITES. IN THE TWO DISTURBANCE SITES. IN THE TWO DISTURBANCE CONTAINING A the hole dispersion has a valley between the antinodal points (2) and (2) and (1) and (1) support  $\mathbb{R}$  is weakly dispersive and  $\mathbb{R}$  $\alpha$  is the susceptibility for such currents is expected since  $\alpha$  $t$ 'ounling  $H(S)$ ' RVE  $\blacksquare$  $n$ in hole dispersion has a valley between the  $n$



# Conclusions *i,j,*

- DF-diagrammatic can be combined with Lattice DQMC to describe doped strongly correlated systems **↓ DE-diagrammatic can be combined with Lattice**  $\overline{\mathbf{5}}$ 
	- Importance of  $t'$  for response on  $d_{x^2-y^2}$  fields and µ dependence shows HTSC-physics  $\int f'$  for response on  $d_{x^2-y^2}$  fields  $\mu$  = *µ* if *i* is a *j* in *i* iii *i* iii *ii* iii *ii* iii *ii* ii *ii*

.<br>Collaborations with:

Sergei Iskakov (Michigan) Evgeny Stepanov (Paris) Mikhail Katsnelson (Nijmegen) *U* Evgeny Stepanov (Paris)<br>Mikhail Katsnelson (Niimegen)



# TB-Model: HTSC



From DFT-calculations: t'/t=-0.3

# 8x8 test DF-QMC vs. DQMC



# AFM vs. Dw





 $0.0 +$ 

0*.*05

 $\begin{array}{|c|c|c|c|c|}\n\hline\n0.05 & & & t_2/t_1 & = 0.2\n\end{array}$ 

 $\delta$ 

 $0.0$   $0.1$   $0.2$ 

*|t*2*/ t*1*|* **=** 0*.*253  $|t_2/t_1| = 0.3$ 

 $\begin{array}{ccc} 0.0 & 0.1 & 0.2 \end{array}$ 

 $\blacktriangledown$ 

the nodal points. Here, we have shown the data calcu-



Ref. [10] by the comparison of *ab initio* result and that