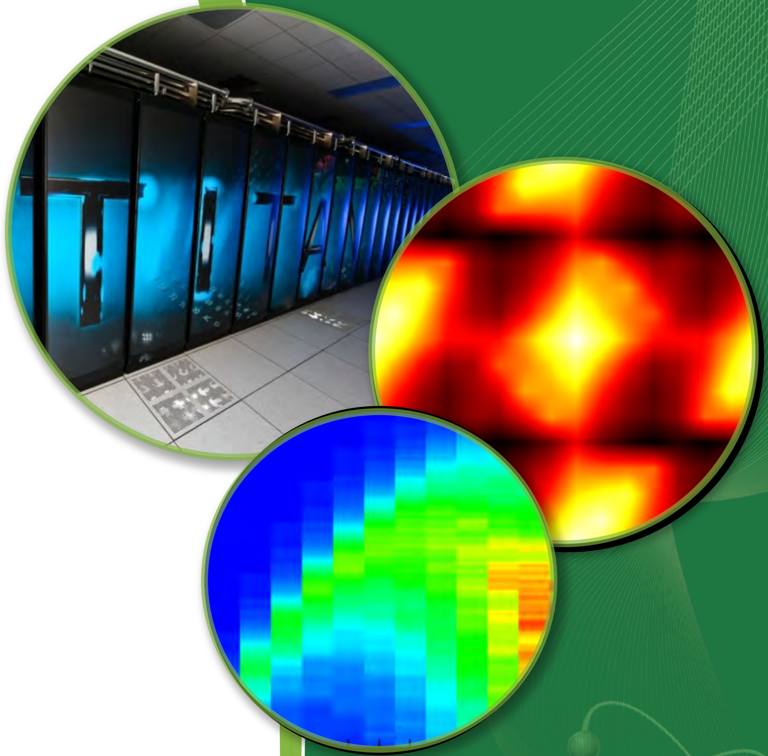
S-wave Pairing from Repulsive Interactions: Quantum Monte Carlo Studies of Systems with Incipient Bands

Thomas A. Maier
Oak Ridge National Laboratory



SciDAC-4 PI meeting, Rockville, MD – July 23, 2018

Outline

- **Introduction of CompFUSE project**
- **Highlights**
- **Pairing in the bilayer Hubbard model near a Lifshitz transition**

CompFUSE: Computational Framework for Unbiased Studies of Correlated Electron Systems – Team

Physics

- **Thomas Maier** (ORNL, Project Director)
- Doug Scalapino (UCSB, co-PI)
- Steven Johnston (UTK, co-PI)
- Satoshi Okamoto (ORNL)
- Gonzalo Alvarez (ORNL)
- Tom Berlijn (ORNL)
- Peizhi Mai (ORNL, postdoc)
- Pontus Laurell (ORNL, postdoc)
- Seher Karakuzu (UTK, postdoc)

Math

- **Feng Bao** (UTC, co-PI)
- **Ed D'Azevedo** (ORNL)
- Clayton Webster (ORNL)
- Xuping Xie (ORNL, postdoc)

Computer Science

- Wael Elwasif (ORNL)
- Ying Wai Li (ORNL)
- Oscar Hernandez (ORNL)
- **Arghya Chatterjee** (ORNL, postmaster)
- Peter Doak (ORNL)

OAK RIDGE National Laboratory | 75 YEARS THE UNIVERSITY OF TENNESSEE KNOXVILLE THE UNIVERSITY OF TENNESSEE CHATTANOOGA UC Santa Barbara

Correlated electron systems

Strong electron-electron interactions

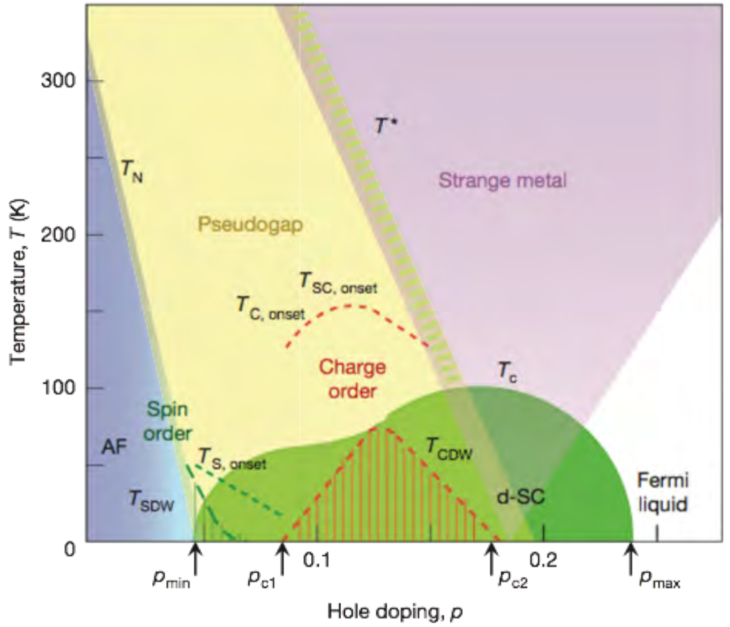
- ***Electrons behave collectively*** and produce ***nearly degenerate*** emergent ***phases***

Unconventional superconductors

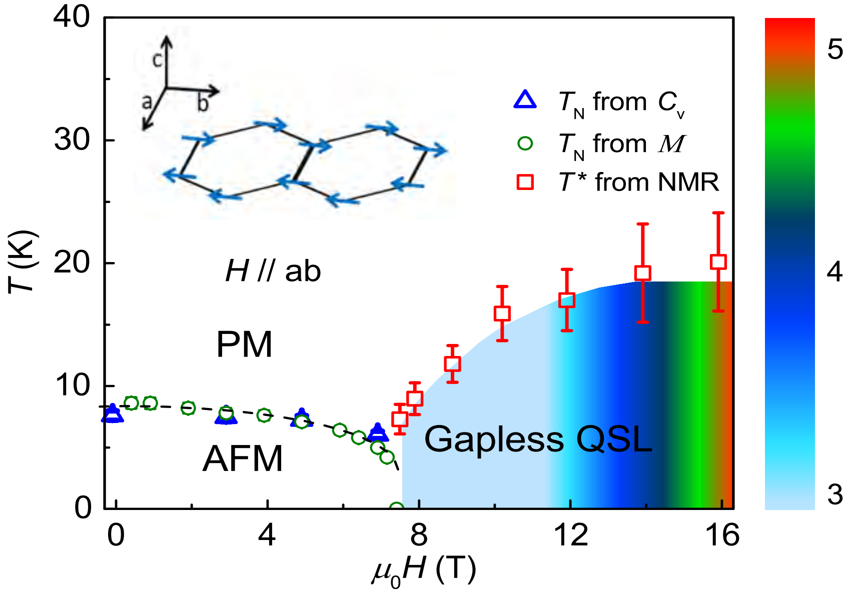
- Cuprates, iron-based superconductors, …
- Magnetism, superconductivity, nematicity, charge order, …
- ***Pairing mechanism?***

Quantum spin liquids

- Geometrically frustrated magnetic interactions
- Honeycomb iridium oxides, ruthenium based materials
- ***Stability of spin liquid ground states?***



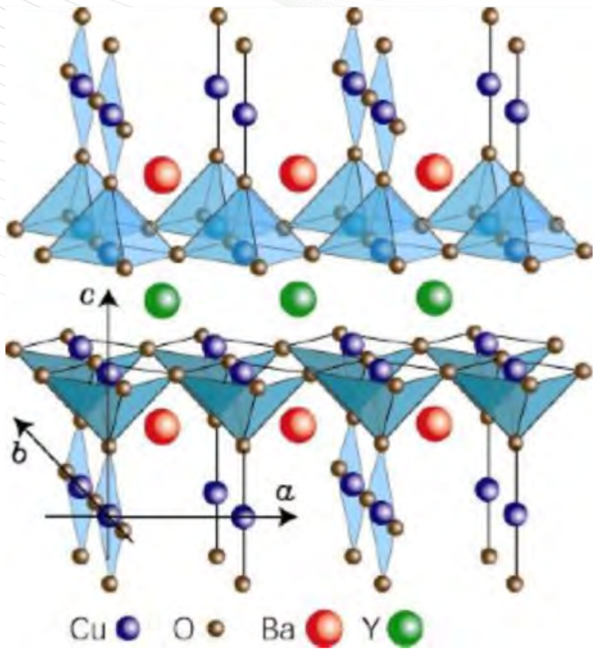
From Keimer et al., Nature '15



From Zheng et al., PRL'17

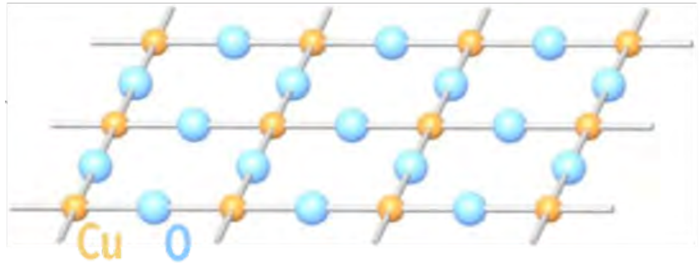
From real materials to reduced models

YBCO

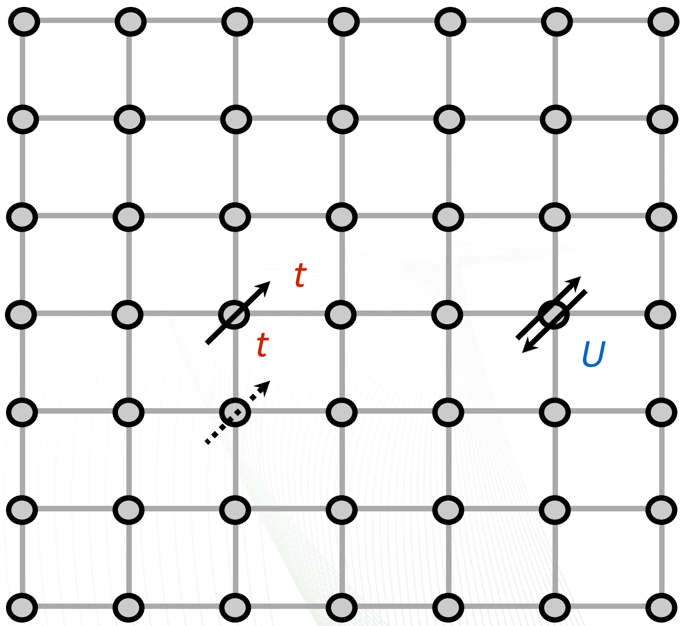


$$\mathcal{H} = -\sum_i \frac{\hbar \nabla_i^2}{2m_e} - \sum_I \frac{\hbar \nabla_I^2}{2M_I} - \sum_{i,I} \frac{Z_I}{|r_i - R_I|} + \frac{1}{2}\sum_{i,I} \frac{1}{|r_i - r_{i'}|} + \frac{1}{2}\sum_{i,I} \frac{Z_I Z_{I'}}{|R_i - R_{i'}|}$$

CuO layer

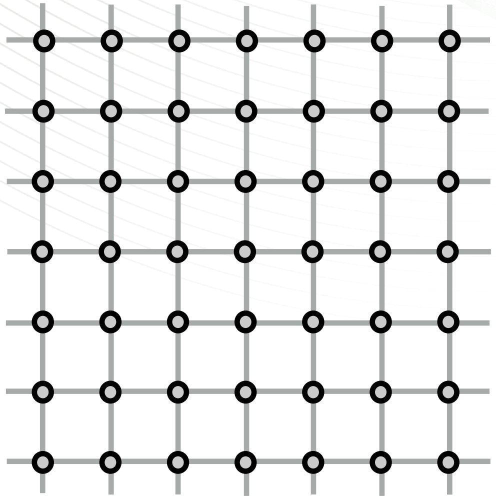


2D Hubbard model

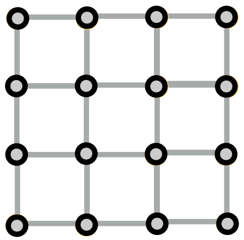


$$\mathcal{H} = \sum_{ij,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

Numerical methods



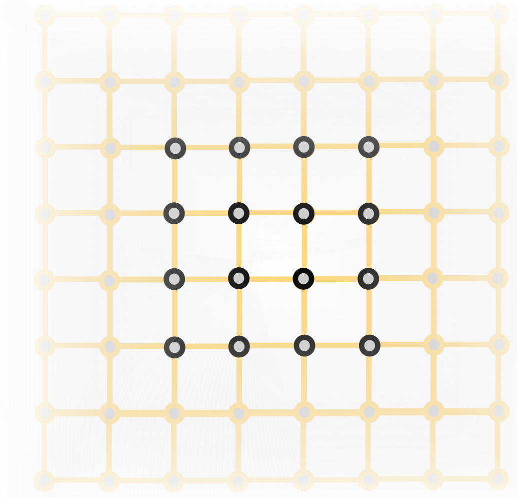
Determinant Quantum Monte Carlo (DQMC)



Blankenbecler et al., PRD '81.

- Finite size cluster
- Monte Carlo sampling of $Z = \mathrm{Tr}e^{-\beta\mathcal{H}}$
- Limited by Fermion sign problem

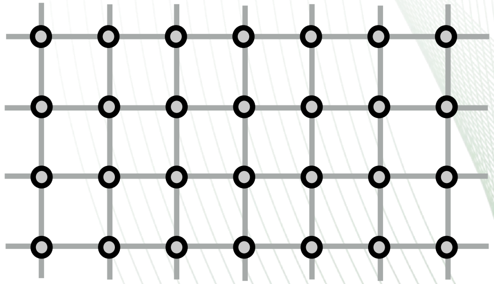
Dynamic Cluster Approximation DCA(QMC)



Maier et al., RMP '05.

- Cluster embedded in self-consistent host
- Monte Carlo sampling of $Z = \int \mathcal{D}[\phi^*\phi]e^{-S[\phi^*,\phi]}$
- Limited by Fermion sign problem (milder)

Density Matrix Renormalization group (DMRG)



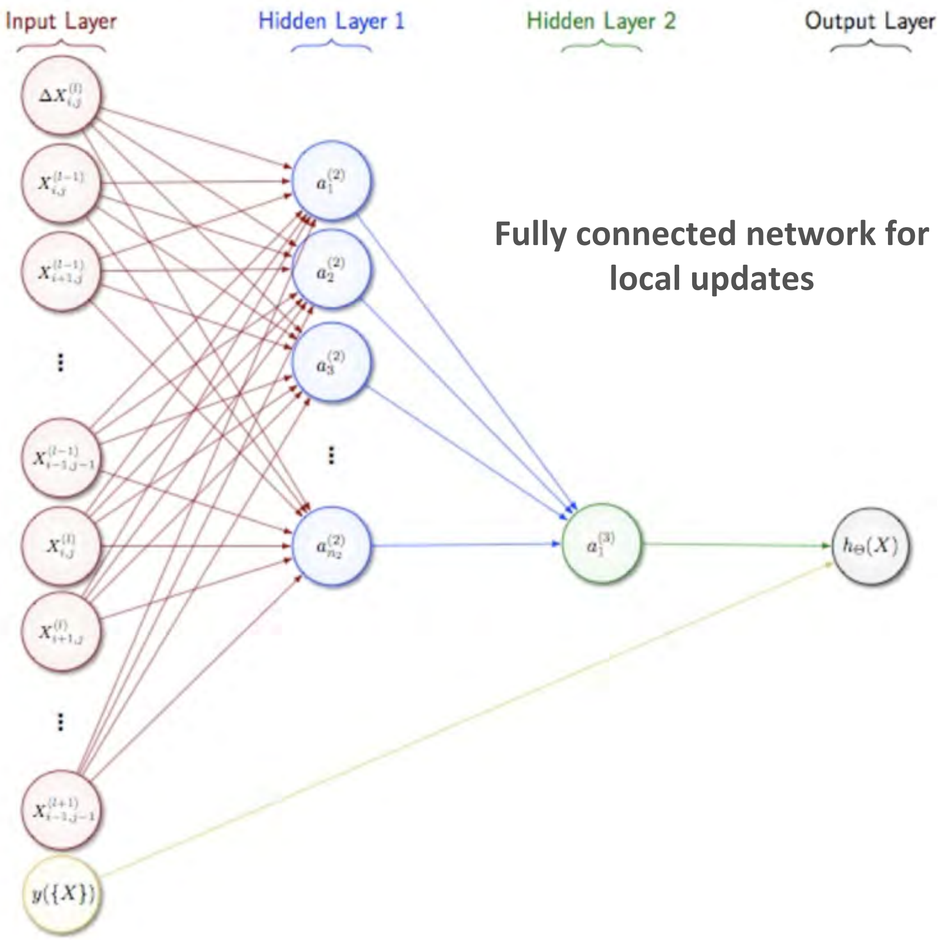
White., PRL '92.

- Finite size, quasi-1D system
- Truncates Hilbert space based on density matrix
- Limited by entanglement entropy

Neural networks to speed up DQMC

DQMC simulations

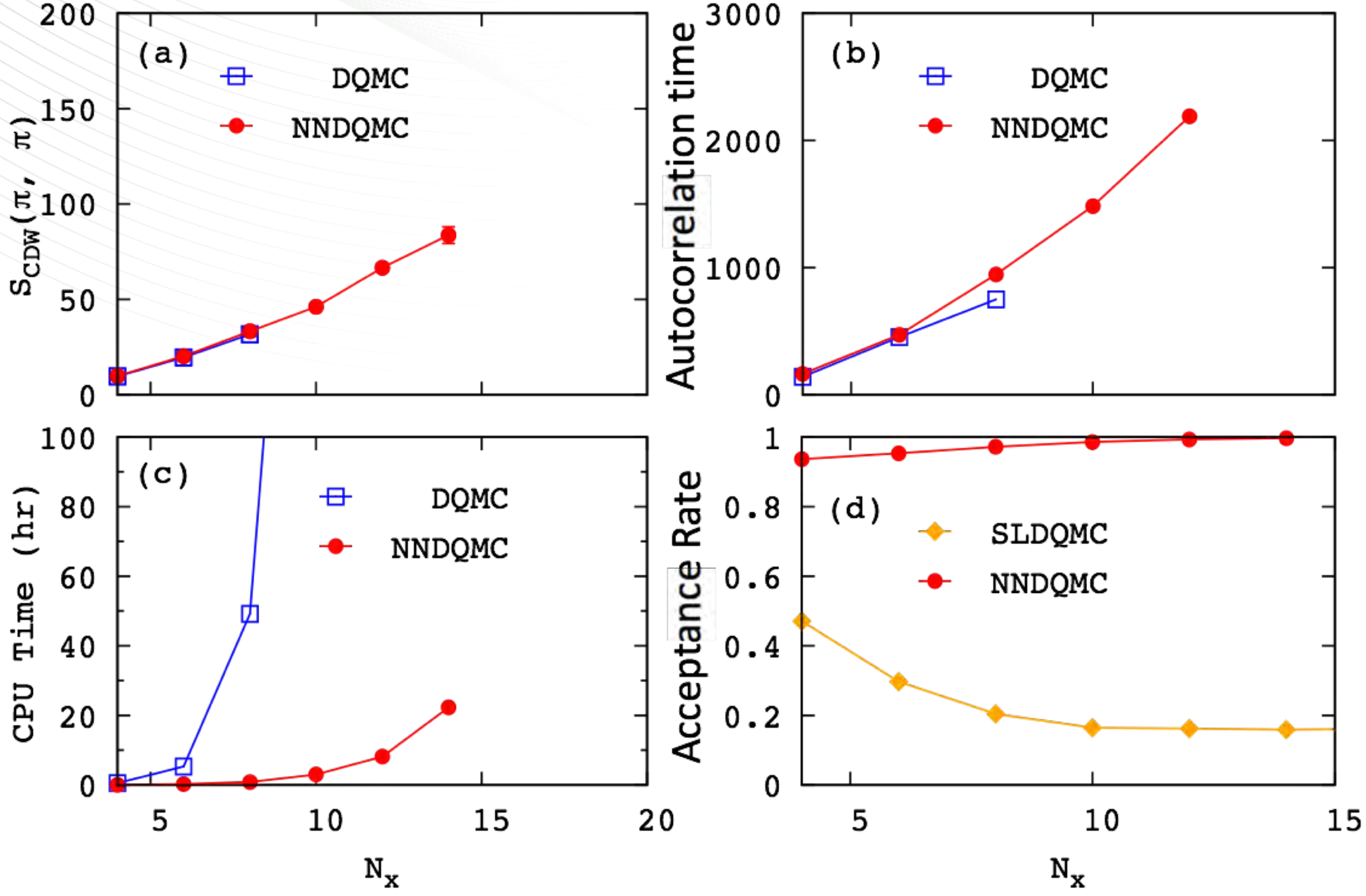
- Local updates requires updating the Green's function at a cost O(N^2)
- Global updates requires recomputing the Green's function from scratch at a cost O(N^3L)
- We trained a ***fully connected neural network*** to predict acceptance probabilities for **local updates** and a ***convolutional neural network*** to predict **global updates**. The only input to the network is the temperature and auxiliary field configurations.
- Many updates can be performed at O(1) cost; the Green's function is recomputed after many cheap updates.
- We train the network using data from a small 4 x 4 lattice, then use the network to sample on a larger system.



Fully connected network for local updates

Neural Network DQMC (NNDQMC) for 2D Holstein model

$$\langle n \rangle = 1, \Omega = t/2, \lambda = t/2$$



NNDQMC simulations with local and global (uniform) updates of the phonon fields

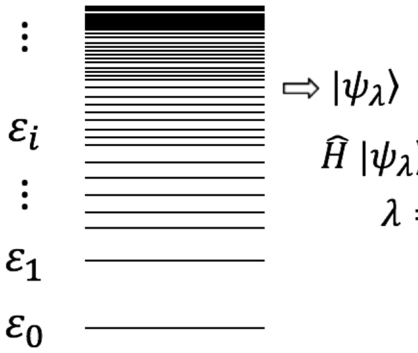
- All parameters were identical between DQMC and NNDQMC simulations such that ***autocorrelation times are comparable***
- Obtained ***identical results*** for both methods.
- ***Full DQMC*** has an effective scaling ***$O(N^{6.8})$***; ***NNDQMC*** has an effective scaling ***$O(N^{4.8})$***.
- Our method maintains **higher acceptance rates** compared to the self-learning method introduced by C. Chen et al., arXiv:1802.06177.

Finite temperature dynamics of interacting quantum models

Thermal pure quantum state - microcanonical Lanczos method

- ***Microcanonical Lanczos method (MCLM)*** is much **more efficient** than finite temperature Lanzcos (FTLM), but needs internal energy $\langle \hat{H} \rangle$ at temperature *T*.
- We propose to use the ***thermal pure quantum state (TPQ)*** to obtain $\langle \hat{H} \rangle$ efficiently, then use MCLM targeting excited state $|\psi_\lambda\rangle$ with energy eigenvalue $\lambda = \langle \hat{H} \rangle$.
- ***TPQ-MCLM*** is **computationally inexpensive** and found to give practically **identical results** to much more expensive FTLM method.
- Future: **DMRG** instead of Lanczos

$\hat{H}\,|\psi_i\rangle = \varepsilon_i|\psi_i\rangle$



$\hat{H}\,|\psi_\lambda\rangle = \lambda|\psi_\lambda\rangle$

$\lambda = \langle \hat{H} \rangle$

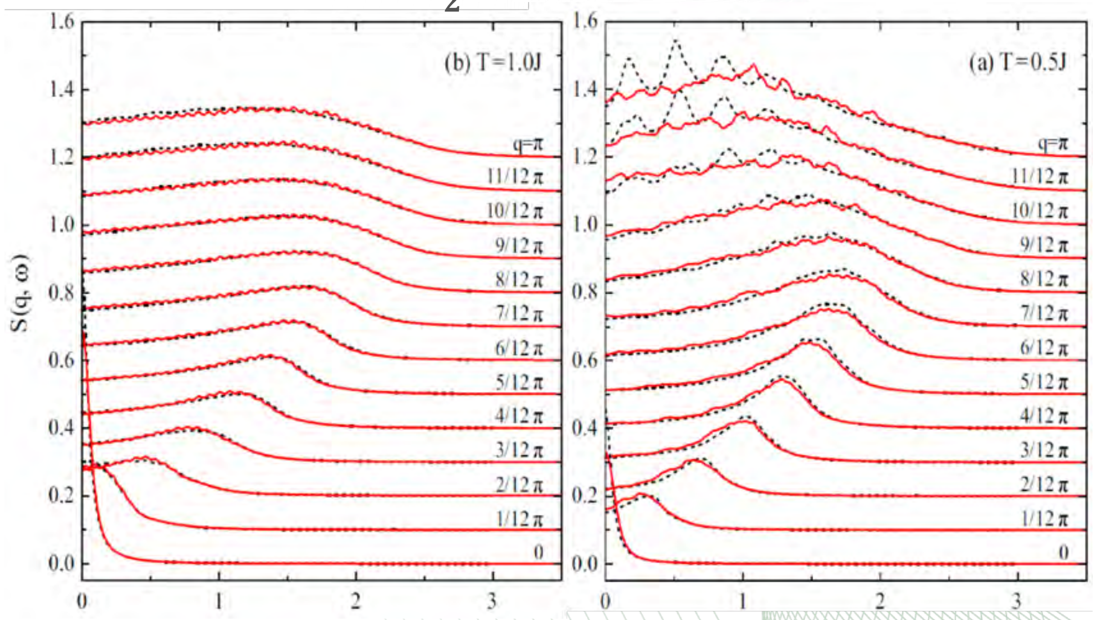
FTLM

$$\langle \hat{A}(t) \rangle = \frac{\sum_i e^{-\varepsilon_i/T} \langle \psi_i | \hat{A}(t) | \psi_i \rangle}{\sum_i e^{-\varepsilon_i/T}}$$

MCLM

$$\langle \hat{A}(t) \rangle = \langle \psi_\lambda | \hat{A}(t) | \psi_\lambda \rangle$$

1D $S = \frac{1}{2}$ Heisenberg chain



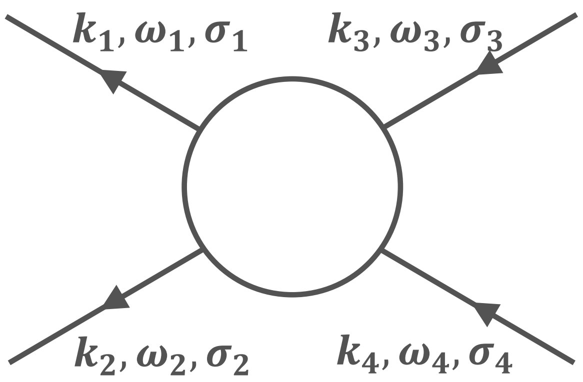
S. Okamoto et al., PRB 83 '18

Oak Ridge National Laboratory

DCA++ on Summit

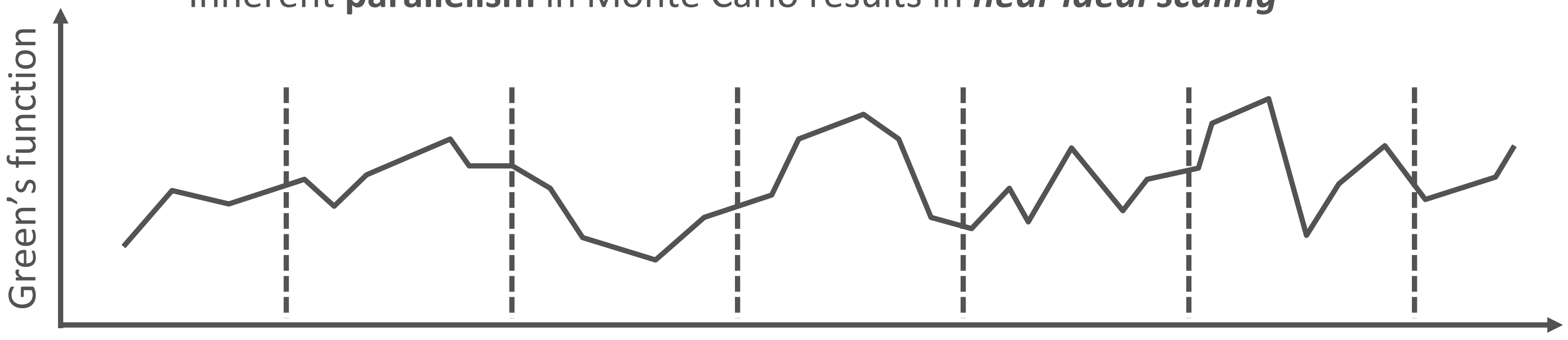
Science objective

- **Efficient calculations** of the ***4-point electron-electron scattering vertex***
- Provides ***deepest insight*** into dominant correlations

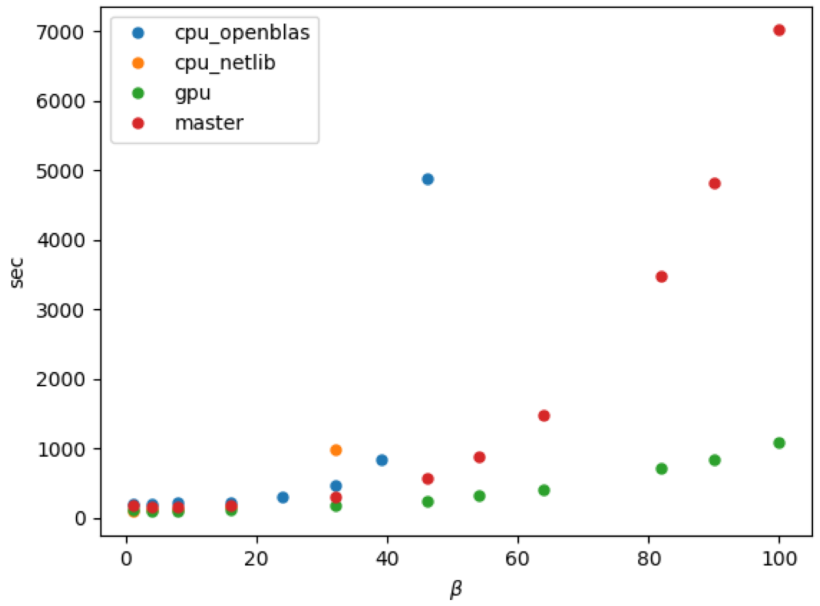


Optimization of DCA++ for Summit

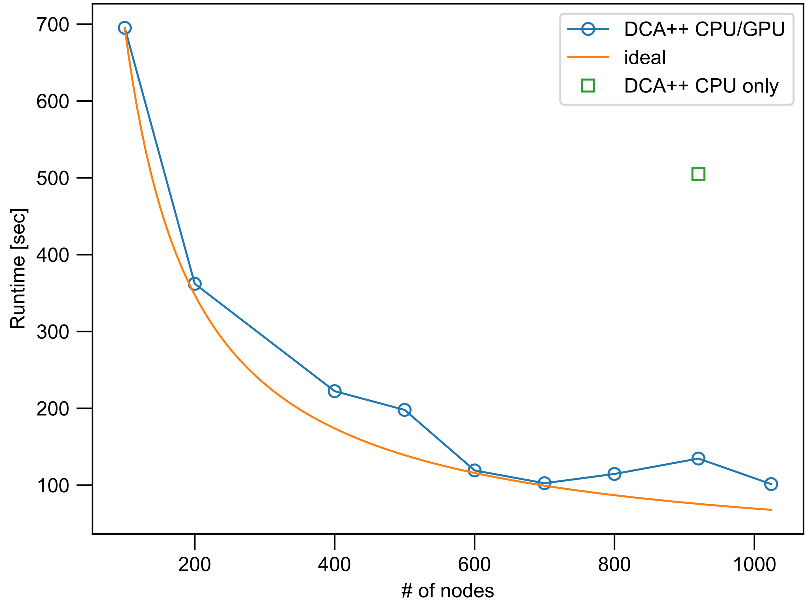
- ***GPU support*** for measurements of **4-point scattering vertex**
- ***Factor 7*** on-node **performance speedup** over previous implementation
- Efficient calculations of the electron-electron scattering vertex
- Inherent **parallelism** in Monte Carlo results in ***near ideal scaling***



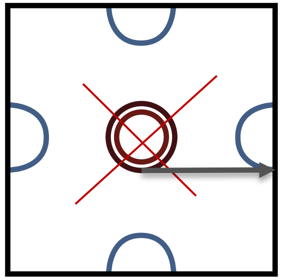
On-node performance



Strong scaling



Pairing in systems with incipient bands: A DCA(QMC) study



Electronic structure of weakly doped iron-SC

- 2 or 3 **hole-pockets and** 2 **electron-pockets**

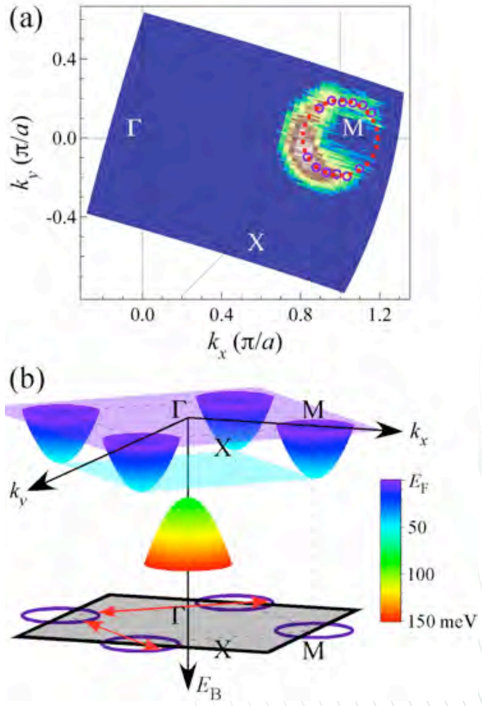
Heavily electron doped iron-SC

- $A_xFe_2Se_2$ (A= K, Rb, Cs; T_c ~ 30 K)
- FeSe monolayer on STO (T_c ~ 60-100 K)
- $(Li_{0.8}Fe_{0.2})OHFeSe$ (T_c ~ 40 K)
- ***Hole bands are ~ 50 – 100 meV below Fermi energy***

Weak coupling studies of pairing in systems with incipient bands

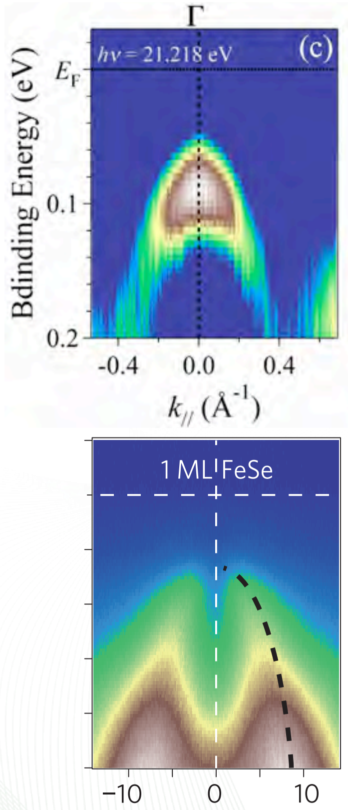
- *Chen et al., PRB '15, Linscheid et al., PRL' 16, Mishra, TAM, Scalapino, Sci. Rep. '16, Leong & Phillips, PRB '16*

$A_xFe_2Se_2$



From Qian et al., PRL '11

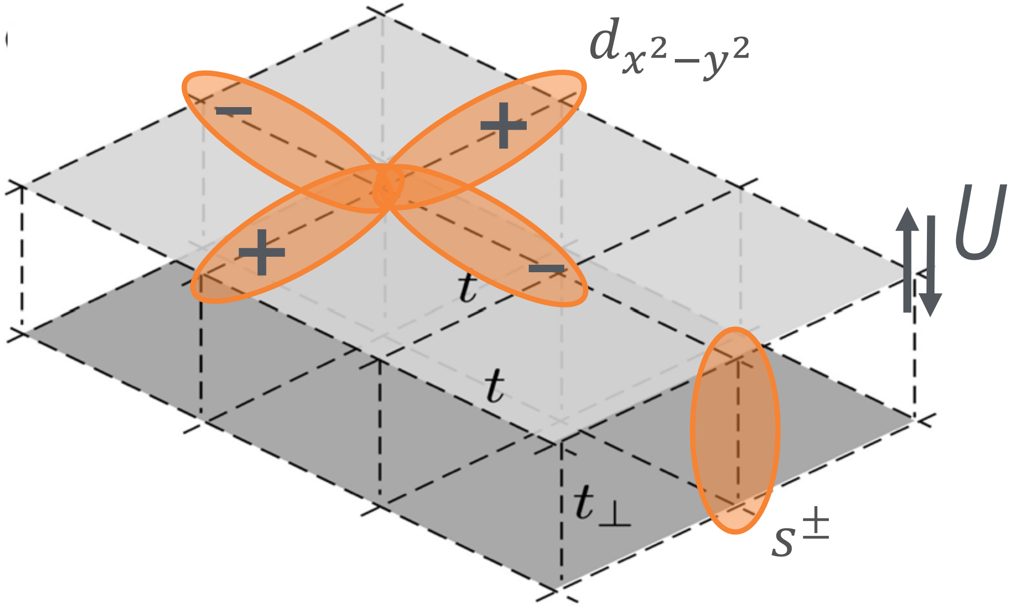
FeSe monolayer

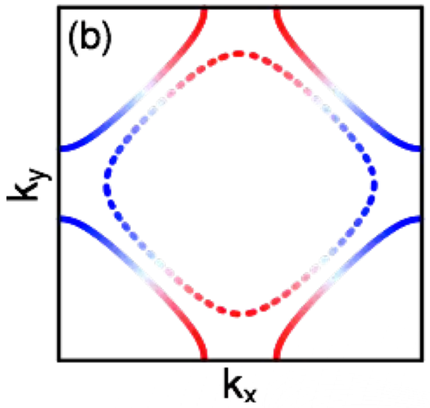


From Tan et al., Nat. Mat. '13

Oak Ridge National Laboratory

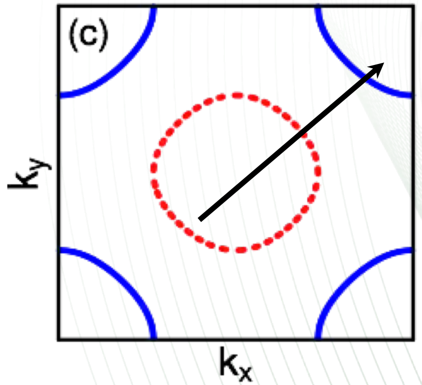
Bilayer Hubbard model and Fe-based superconductors





$\frac{t_\perp}{t} = 0.5$

$$\Delta(k) = \Delta_0\,(\cos k_x - \cos k_y)$$

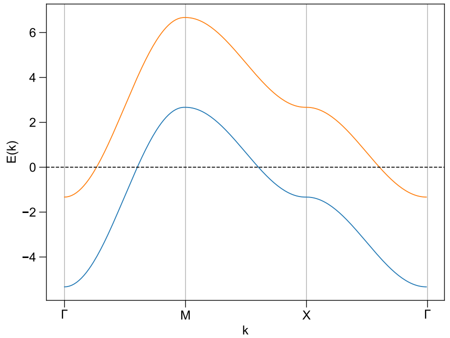


$\frac{t_\perp}{t} = 2.0$

$$\Delta(k) = \Delta_0 \cos k_z$$

$$\epsilon_k = -2t(\cos k_x + \cos k_y) - t_\perp \cos k_z$$

→ **Bonding and anti-bonding bands**



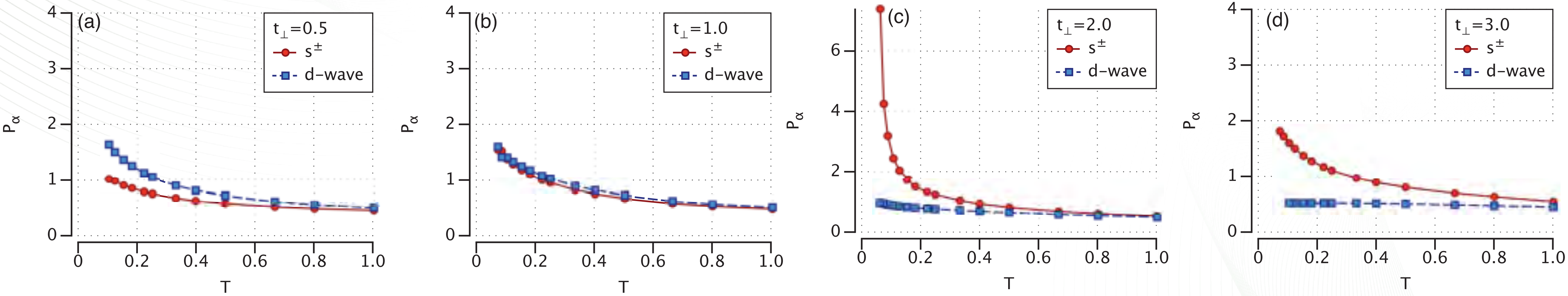
TAM & D.J. Scalapino, PRB 83 '11

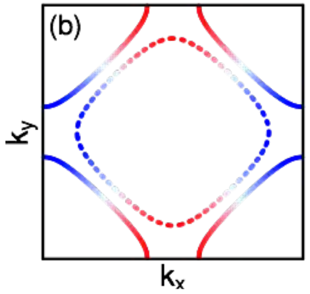
Bilayer with 2 Fermi pockets

TAM & D.J. Scalapino, PRB 83 '11

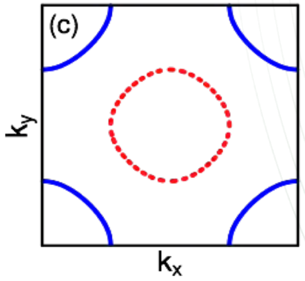
$$P_\alpha(T) = \int_0^\beta d\tau \langle \Delta_\alpha(\tau)\Delta_\alpha^\dagger(0)\rangle$$

$U = 6t, \langle n\rangle = 0.95; (4\times4)\times2$ cluster





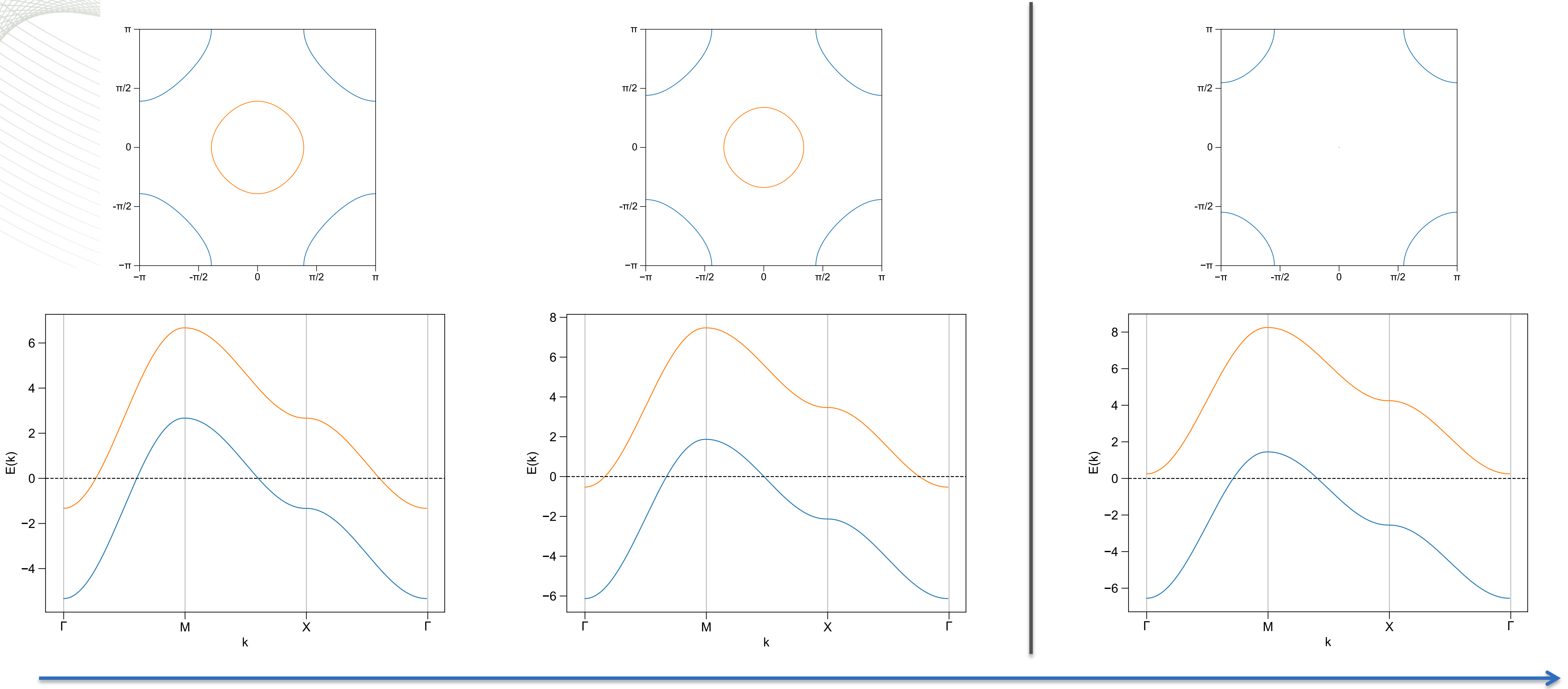
$\Delta(k) = \Delta_0\,(\cos k_x - \cos k_y)$



$\Delta(k) = \Delta_0 \cos k_z$

Taking the bilayer through a Lifshitz transition

Lifshitz transition



Increasing $t_\perp$

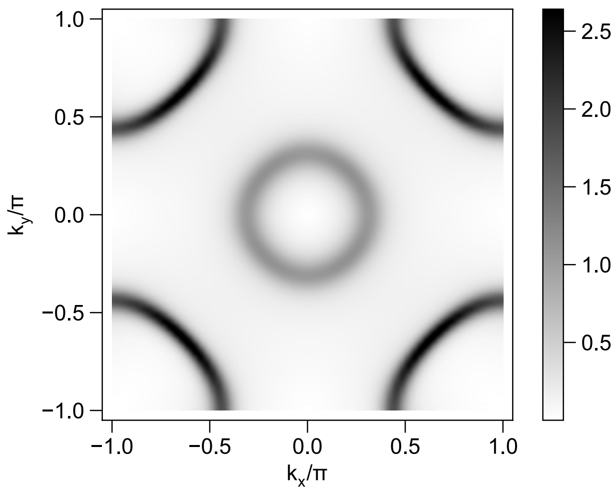
Bilayer with 1 Fermi pocket and incipient band

$U = 8t, \langle n \rangle = 0.85$; $(4\times4)\times2$ cluster

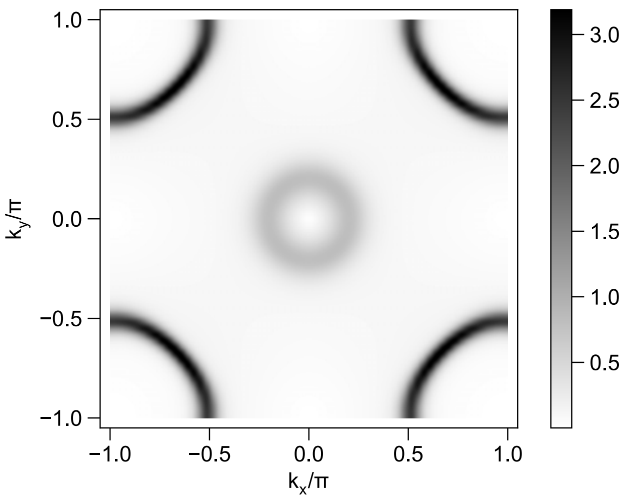
Lifshitz transition

$|\nabla n(k)|$

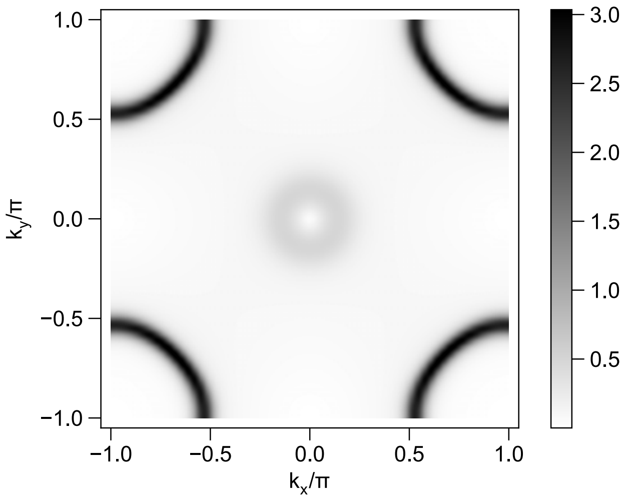
$t_\perp = 2.0$



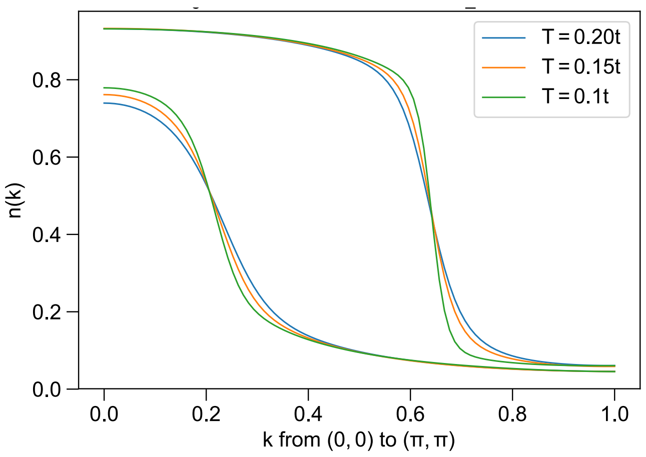
$t_\perp = 2.3$

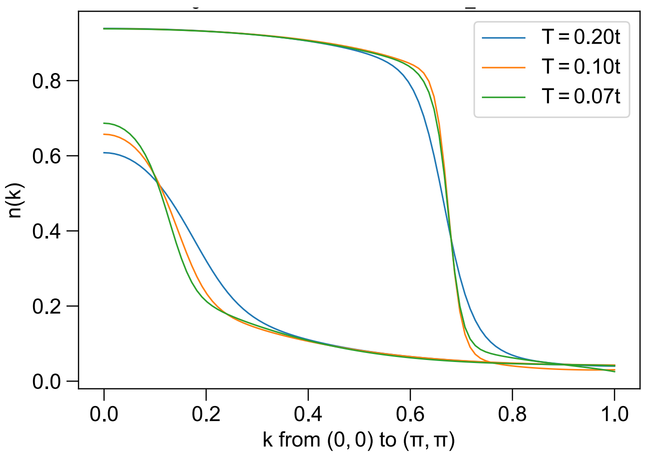


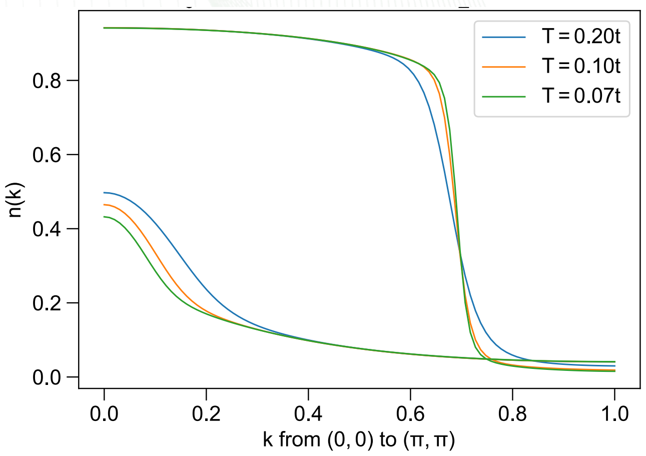
$t_\perp = 2.45$



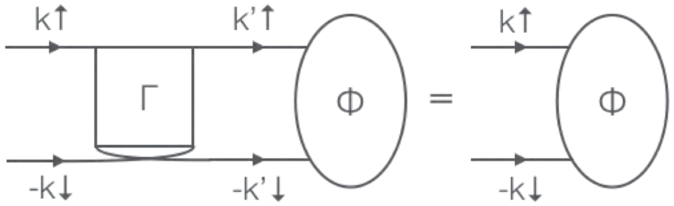
$n(k)$ along 0 → (π,π)







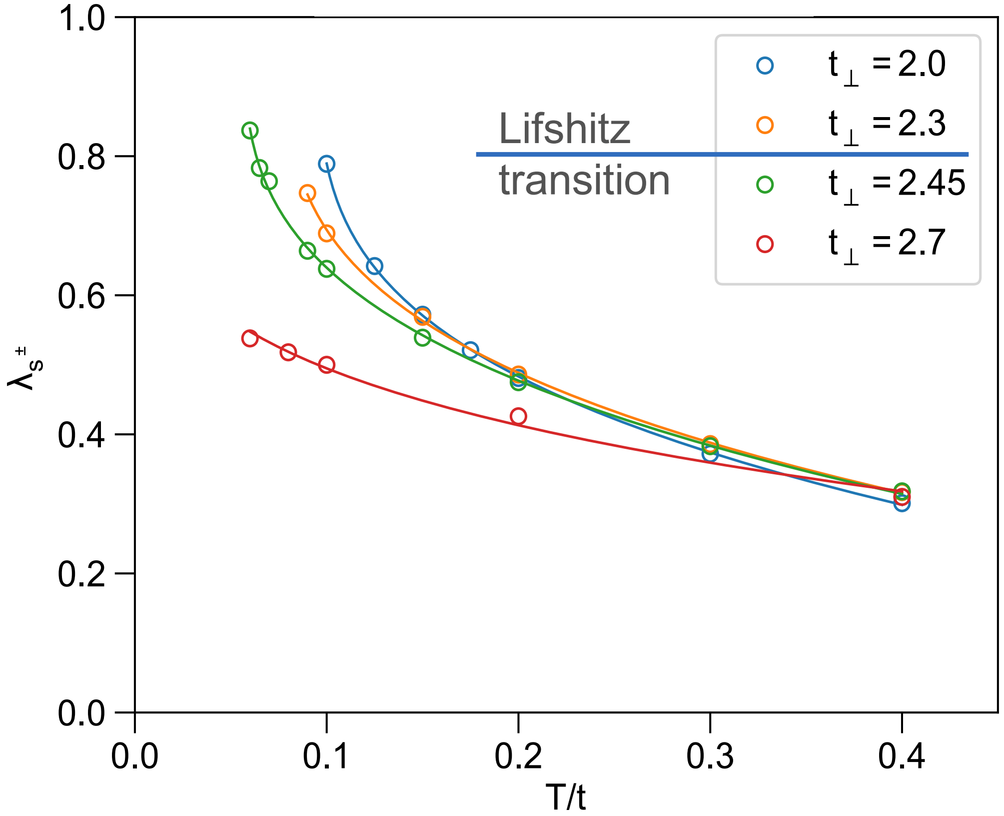
Leading $s^{\pm}$ pairing state



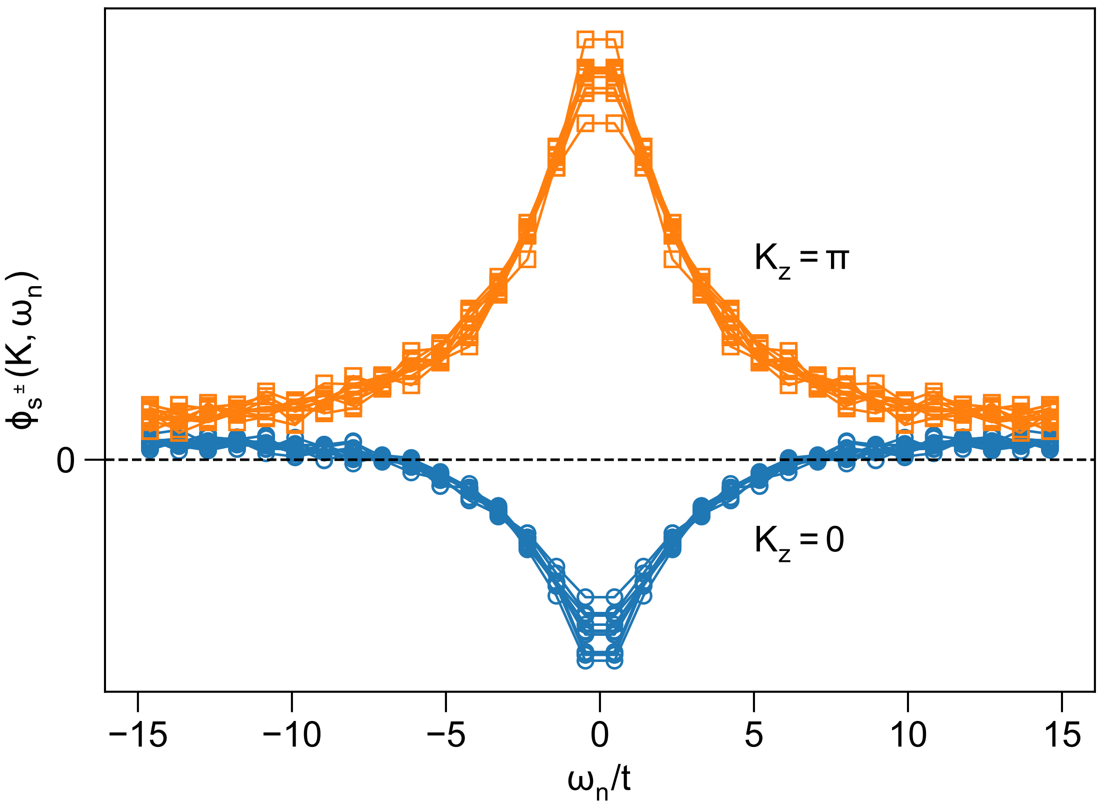
Eigenvalues and –vectors of Bethe-Salpeter equation (linearized, fully renormalized gap equation)

$$-\frac{T}{N}\sum_{k'}\Gamma(k,k')G(k')G(-k')\phi_\alpha(k') = \lambda_\alpha\phi_\alpha(k)$$

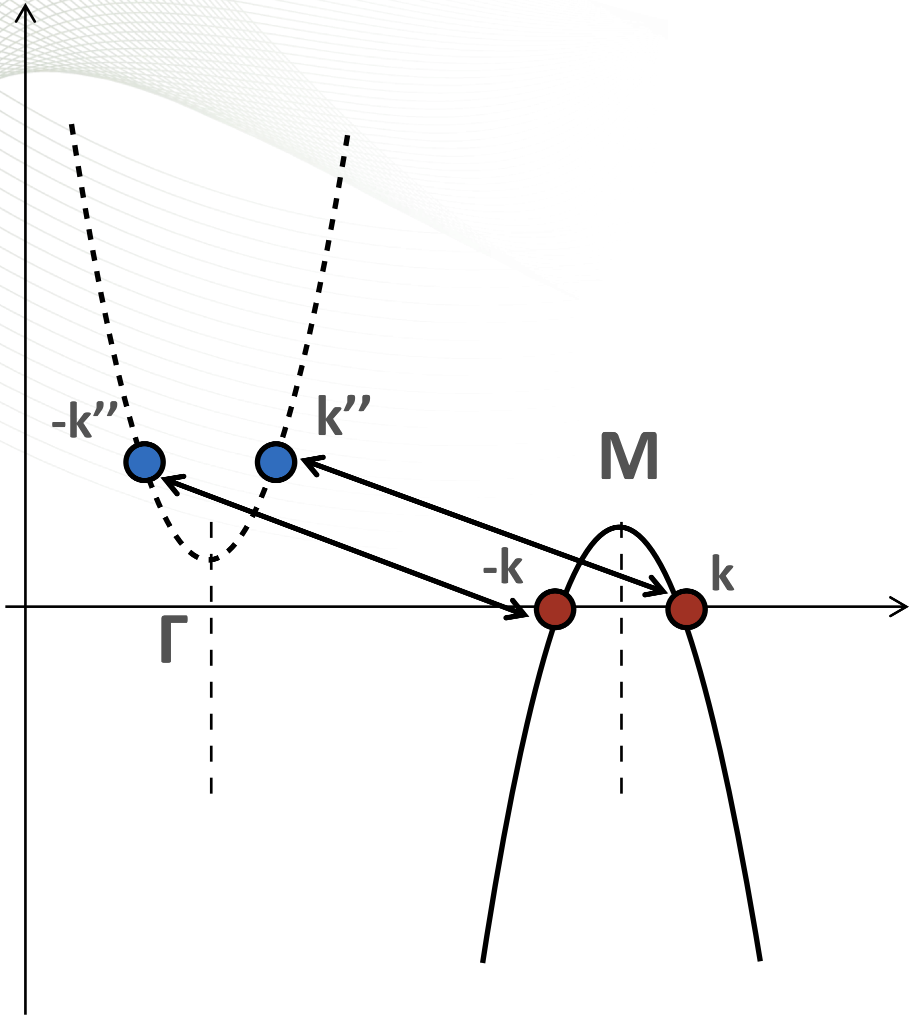
$s^{\pm}$ eigenvalue



$s^{\pm}$ eigenvector for $t_\perp = 2.45t$

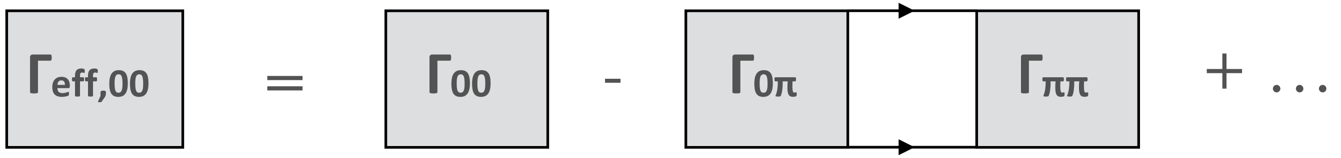


Effective pair scattering on active band



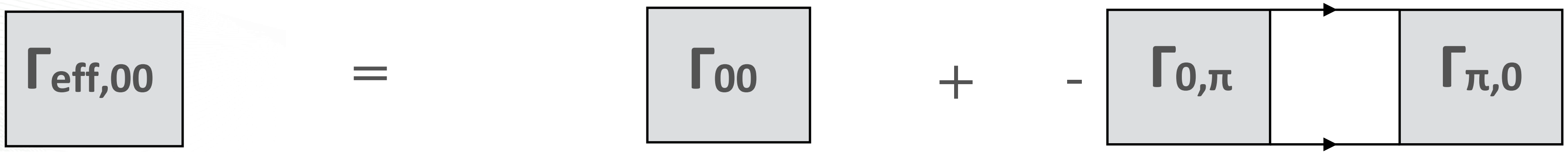
$$-\frac{T}{N}\begin{pmatrix}\Gamma_{00}G_0G_0 & \Gamma_{0\pi}G_\pi G_\pi \\ \Gamma_{\pi 0}G_0G_0 & \Gamma_{\pi\pi}G_\pi G_\pi\end{pmatrix}\begin{pmatrix}\phi_0 \\ \phi_\pi\end{pmatrix} = \lambda\begin{pmatrix}\phi_0 \\ \phi_\pi\end{pmatrix}$$

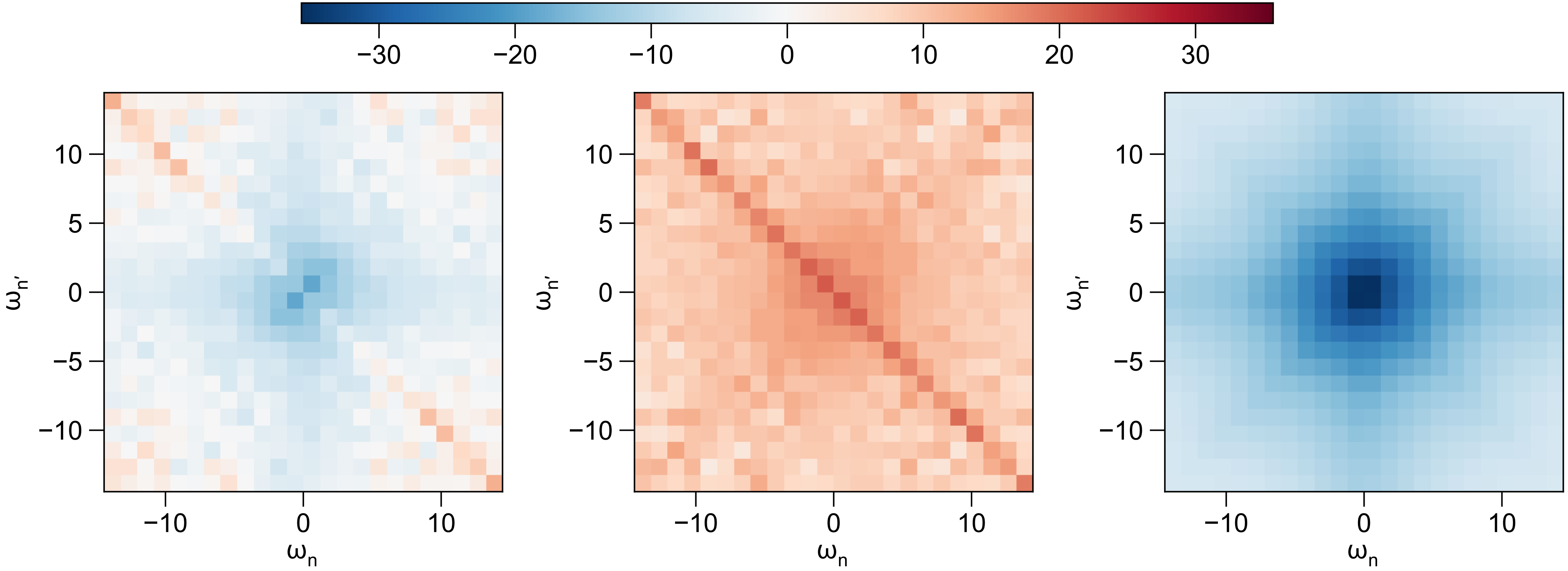
Usual repulsive interaction on hole band including local Coulomb interaction



Additional attractive interaction from virtual pair scattering to unoccupied electron-band

QMC results for effective interaction





Effective interaction **Repulsive** **Attractive**

Summary & Conclusions

CompFUSE project

- **DQMC, DCA(QMC)** and **DMRG** algorithm development
- Simulations of **unconventional superconductors** and **quantum spin liquids**
- Focus on **dynamics** and **4-point scattering vertex**

Pairing in systems with incipient bands

- DCA(QMC) study of **bilayer Hubbard model** with **incipient band**
- Dominant **pairing** correlations are ***s*-wave**
- Gap on incipient band has opposite sign and larger magnitude than gap on Fermi surface
- Virtual pair scattering to incipient band gives **effectively attractive pairing interaction** for Fermi surface states

This work was supported by the Scientific Discovery through Advanced Computing (SciDAC) program funded by U.S. Department of Energy, Office of Science, Advanced Scientific Computing Research and Basic Energy Sciences, Division of Materials Sciences and Engineering.