Dynamical Mean Field and Dynamical Cluster Approximation Based Theory of Superconductivity

Thomas A. Maier

Oak Ridge National Laboratory

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OUTLINE

- **Superconductivity – Introduction**
- **DMFT & Dynamic Cluster Approximation**
- **Superconductivity in 2D Hubbard model**

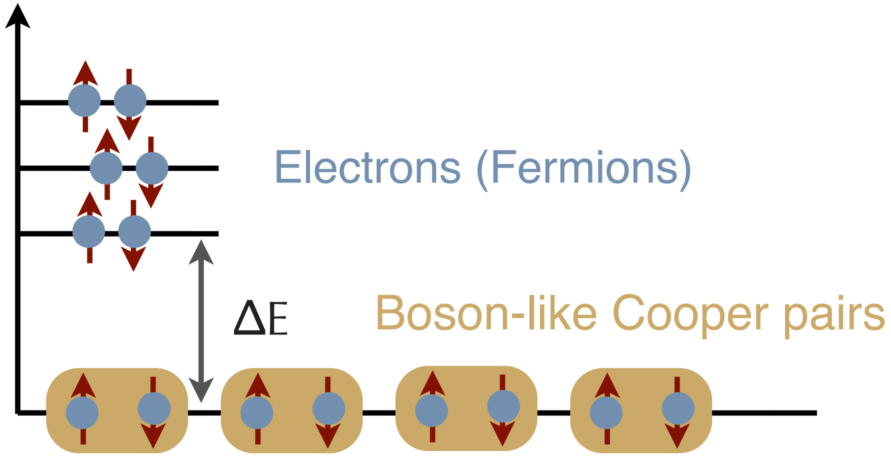
Superconductivity – the Basics

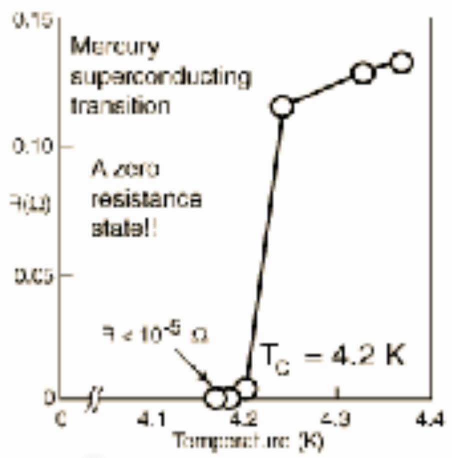
Phenomenology

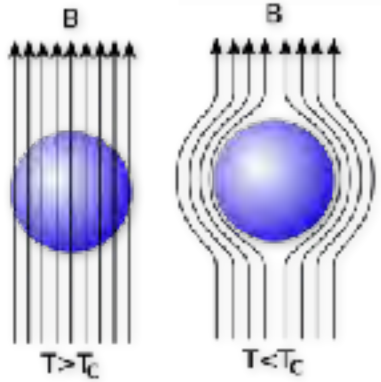
- First discovered in Hg by Kamerlingh Onnes (1911)
- Perfect conductivity (zero resistance)
- Perfect diamagnetism (Meissner-Ochsenfeld effect, 1933)
  ⟶ implies collective behavior of electrons

Microscopic theory

- Electrons in time-reversed momentum states from spin-singlet boson-like Cooper pairs
- Cooper pairs condense into macroscopic quantum state

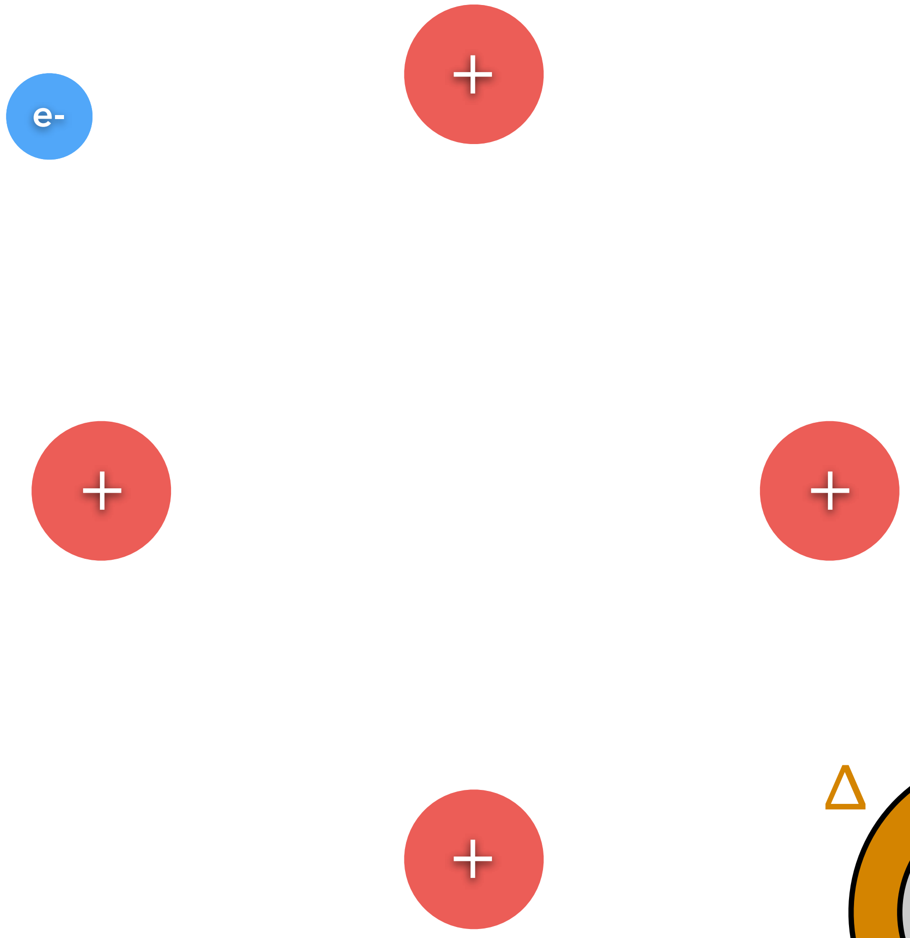






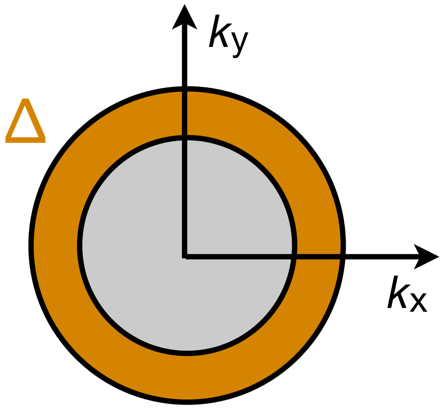
Bardeen Cooper Schrieffer

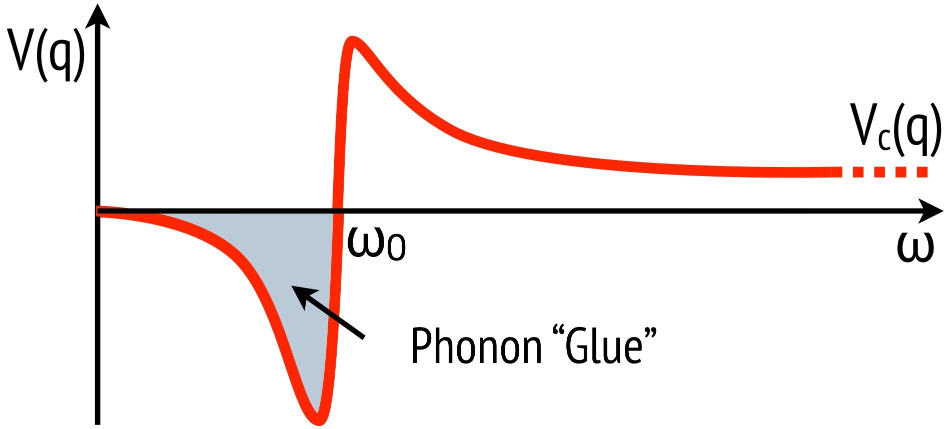
Pair Formation in Conventional Superconductors



Phonon mechanism

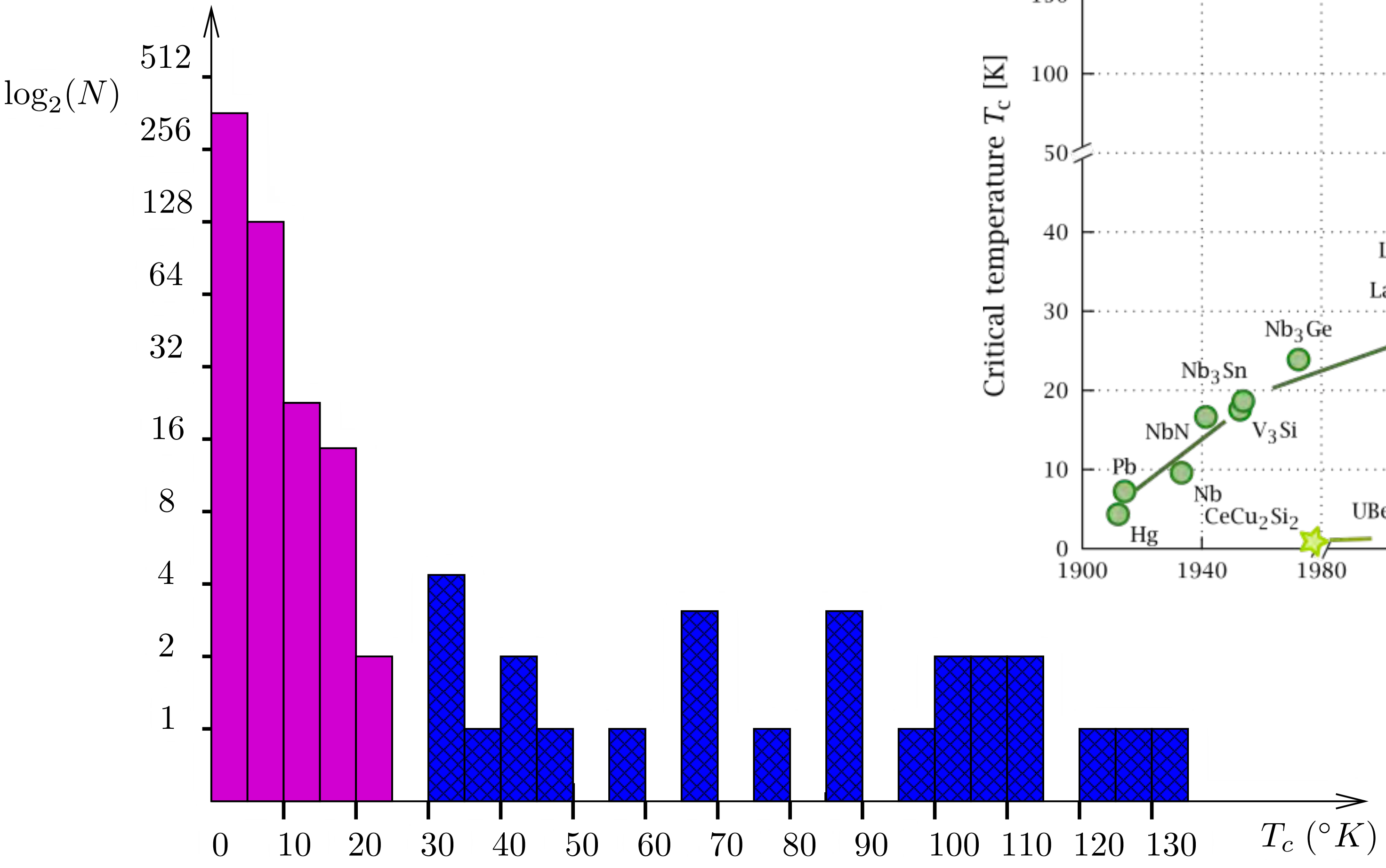
- Local in space: Cooper pair wave-function has s-wave symmetry
- Retarded in time (ion dynamics slow compared to electrons)
- Retardation limits T_C ($T_C \ll \omega_0$)



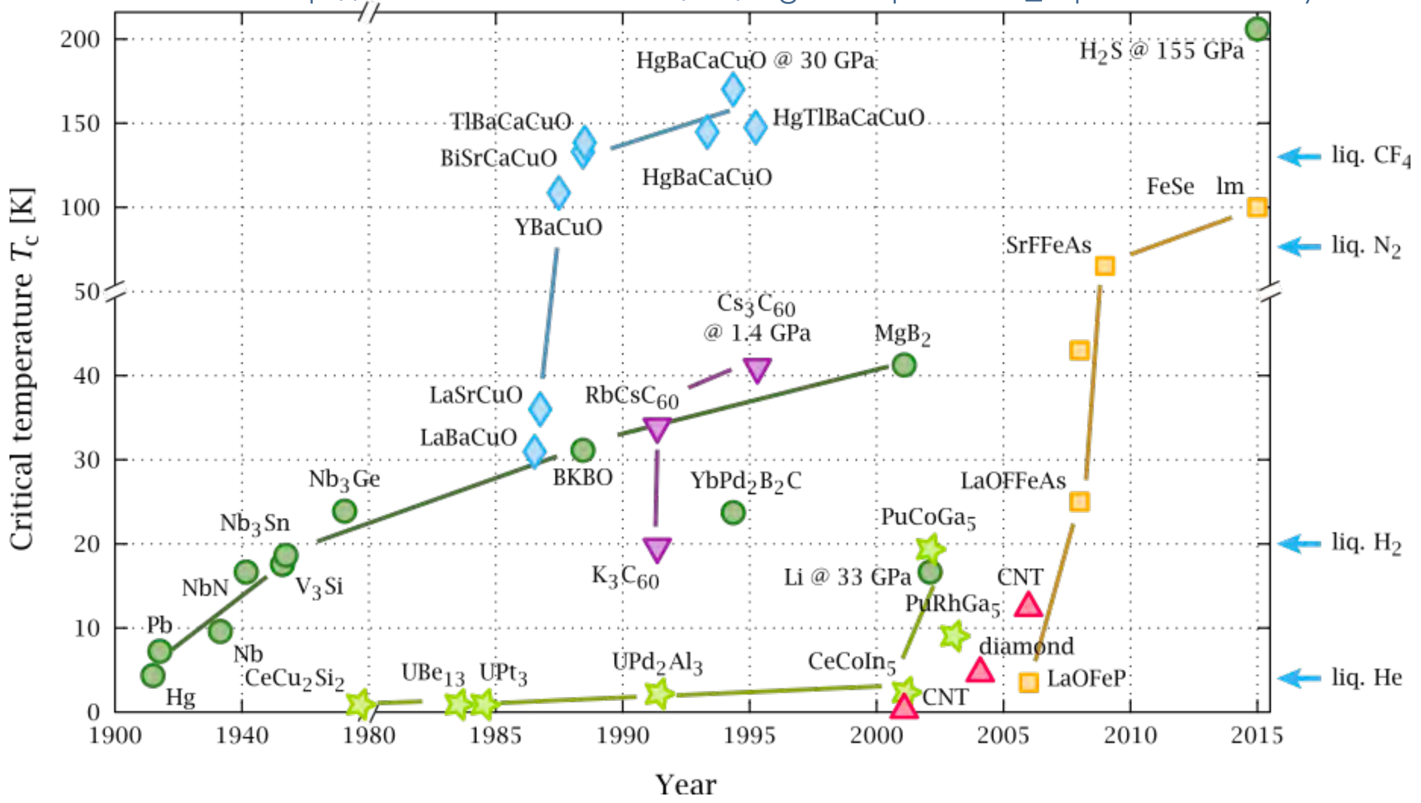


Materials Progress

Credit: http://www.wikiwand.com/en/High-temperature_superconductivity



Kivelson & Fradkin '05

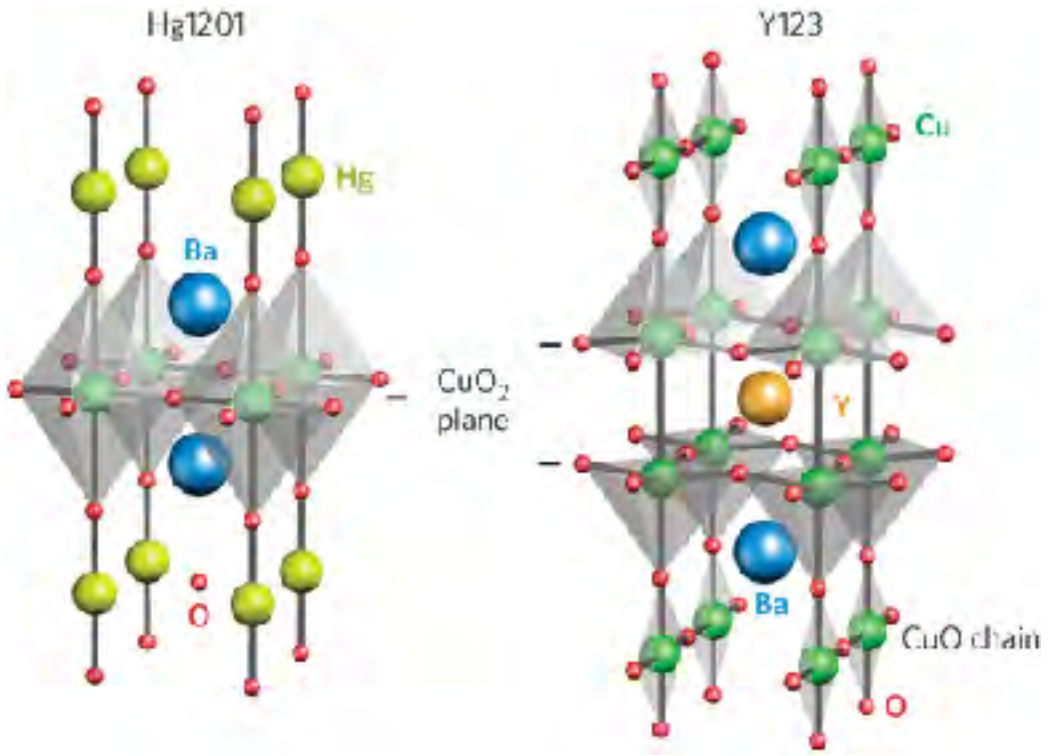


Conventional (BCS) superconductors

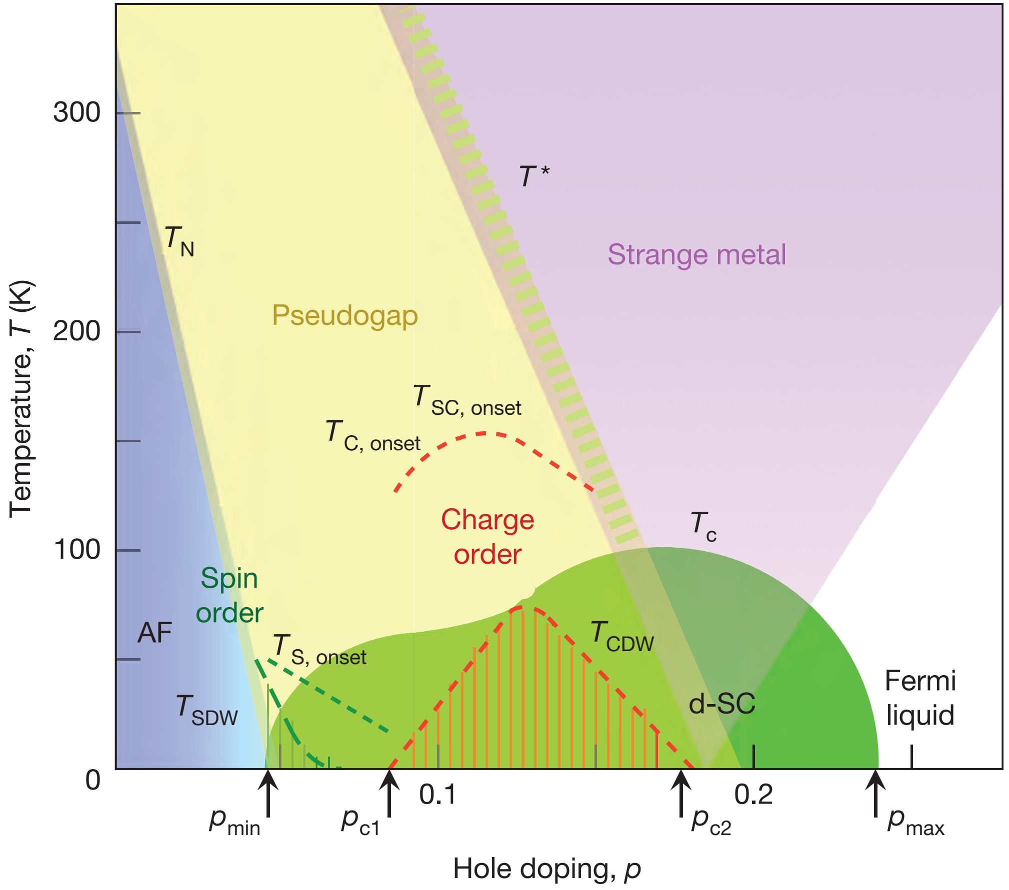
Unconventional superconductors

"Superconductivity is everywhere but sparse" Z. Fisk et al., Phil. Mag. '09

Cuprates



Barišić et al., Nat. Phys. '13

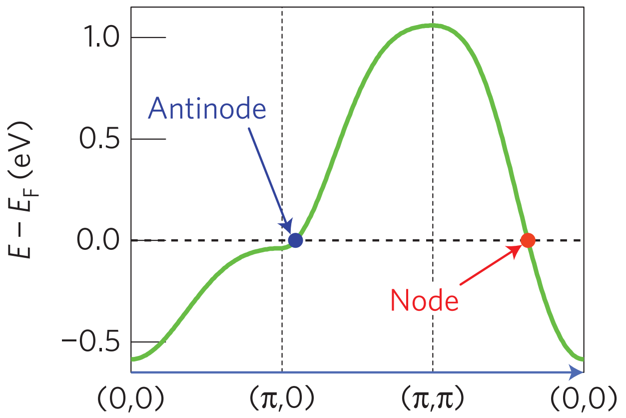


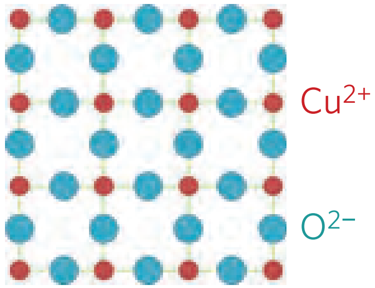
Keimer et al., Nature '15

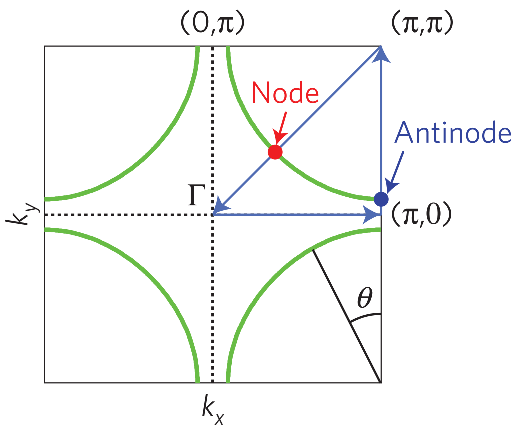
"If one looks hard enough, one can find in the curates something that is reminiscent of almost any interesting phenomenon in solid state physics."

Kivelson & Yao, Nat. Mat. '08

Cuprates: Electronic Structure & Hubbard Model



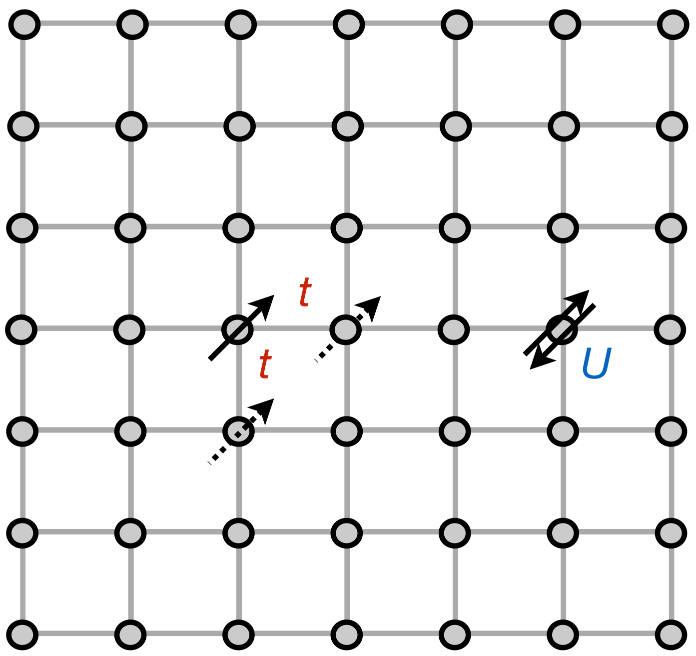




Hashimoto et al., Nat. Phys. '14

Anderson, Science '87

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



DMFT and Dynamic Cluster Approximation (DCA)

Preliminary Remarks

Thermodynamic Green's function

$$G_{ij,\sigma} = -\langle T_\tau c_{i\sigma}(\tau) c^\dagger_{j\sigma}\rangle$$

$$G_{ij,\sigma}(i\omega_n) = \int_0^\beta d\tau\, e^{i\omega_n\tau} G_{ij,\sigma}(\tau)\,,\ \omega_n = (2n+1)\pi T$$

$$G_\sigma(\mathbf{k}, i\omega_n) \equiv \langle\langle c_{\mathbf{k},\sigma}; c^\dagger_{\mathbf{k},\sigma}\rangle\rangle_{i\omega_n} = \frac{1}{N}\sum_{ij} e^{i\mathbf{k}(\mathbf{r}_i - \mathbf{r}_j)} G_{ij,\sigma}(i\omega_n)$$

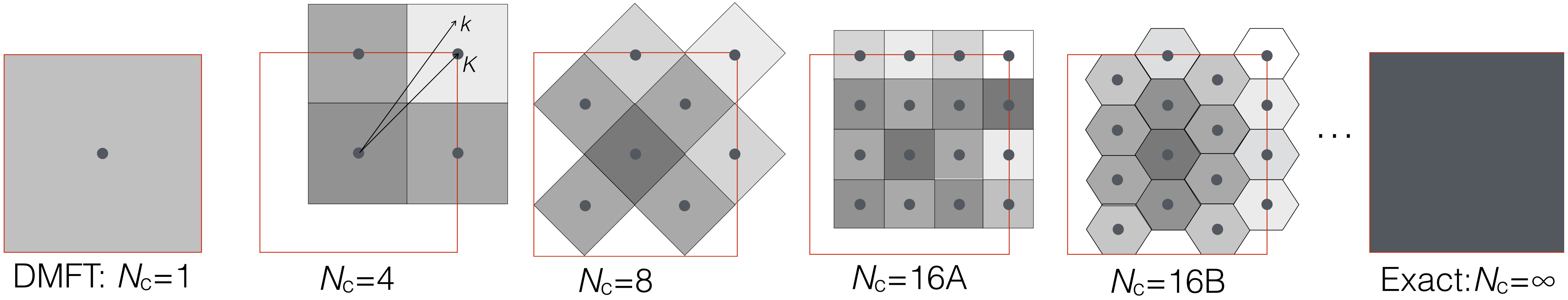
Non-interacting (*U*=0) Green's function

$$G_0(\mathbf{k}, i\omega_n) = \frac{1}{i\omega_n + \mu - \varepsilon_\mathbf{k}}\,;\ \ \varepsilon_\mathbf{k} = -2t(\cos k_x + \cos k_y)$$

Interacting Green's function

$$G(\mathbf{k}, i\omega_n) = \frac{1}{G_0^{-1}(\mathbf{k}, i\omega_n) - \Sigma(\mathbf{k}, i\omega_n)}$$

Dynamic Cluster Approximation (DCA) & DMFT



General idea

- Represent bulk system by a reduced number of cluster degrees of freedom, and use coarse-graining to retain information about remaining degrees of freedom

Self-energy approximation

$\Sigma(\mathbf{k}, i\omega_n) \simeq \Sigma_c(\mathbf{K}, i\omega_n)$ (in DCA)

$\Sigma(\mathbf{k}, i\omega_n) \simeq \Sigma_{ii}(i\omega_n)$ (in DMFT)

Hettler *et al.*, PRB '98
Maier *et al.*, RMP '05

DCA (DMFT) Self-Consistency

(1) Coarse-graining

$$\bar{G}(\mathbf{K}, i\omega_n) = \frac{N_c}{N} \sum_{\mathbf{k} \in \mathscr{P}_{\mathbf{K}}} G(\mathbf{k}, i\omega_n) = \frac{N_c}{N} \sum_{\mathbf{k} \in \mathscr{P}_{\mathbf{K}}} \frac{1}{i\omega_n - \varepsilon_{\mathbf{k}} + \mu - \Sigma_c(\mathbf{K}, i\omega_n)}$$

(2) Cluster exclusion

$$\mathscr{G}_0(\mathbf{K}, i\omega_n) = \left[\bar{G}^{-1}(\mathbf{K}, i\omega_n) + \Sigma_c(\mathbf{K}, i\omega_n)\right]^{-1}$$

(3) Cluster problem solution

$$S[\phi^*, \phi] = -\int_0^\beta d\tau \int_0^\beta d\tau' \sum_{ij,\sigma} \phi^*_{i\sigma}(\tau) \mathscr{G}_{0,ij,\sigma}(\tau - \tau') \phi_{j\sigma}(\tau) + \int_0^\beta d\tau \sum_i U \phi^*_{i\uparrow}(\tau) \phi_{i\uparrow} \phi^*_{i\downarrow}(\tau) \phi_{i\downarrow}(\tau)$$

$$G_{c,ij,\sigma}(\tau - \tau') = \frac{1}{Z} \int \mathscr{D}[\phi^* \phi] \phi_{i\sigma}(\tau) \phi^*_{j\sigma}(\tau') e^{-S[\phi^*, \phi]} \; ; \; Z = \int \mathscr{D}[\phi^* \phi] e^{-S[\phi^*, \phi]}$$

(4) New self-energy

$$\Sigma_c(\mathbf{K}, i\omega_n) = \mathscr{G}_0^{-1}(\mathbf{K}, i\omega_n) - G_c^{-1}(\mathbf{K}, i\omega_n)$$

Nambu-Gorkov Formalism for Superconducting State

Superconducting order parameter

$$\Delta_{\mathbf{k}} = \langle c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow} \rangle \neq 0 \text{ for some } \mathbf{k}$$

Anomalous Green's function

$$F(\mathbf{k}, i\omega_n) = \langle\langle c_{\mathbf{k}\uparrow}; c_{-\mathbf{k}\downarrow} \rangle\rangle_{i\omega_n}$$

Nambu spinors

$$\Psi^\dagger_{\mathbf{k}} = \left(c^\dagger_{\mathbf{k}\uparrow}, c_{-\mathbf{k}\downarrow} \right) \quad ; \quad \Psi_{\mathbf{k}} = \begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c^\dagger_{-\mathbf{k}\downarrow} \end{pmatrix}$$

Green's function matrix

$$\mathbf{G}(\mathbf{k}, i\omega_n) = \langle\langle \Psi_{\mathbf{k}}; \Psi^\dagger_{\mathbf{k}} \rangle\rangle_{i\omega_n} = \begin{pmatrix} G(\mathbf{k}, i\omega_n) & F(\mathbf{k}, i\omega_n) \\ F^*(\mathbf{k}, -i\omega_n) & -G^*(\mathbf{k}, i\omega_n) \end{pmatrix}$$

Symmetry	$\Delta_{\mathbf{k}}$
s-wave	const.
Extended *s*–wave	$\cos k_x + \cos k_y$
$d_{x^2-y^2}$ – wave	$\cos k_x - \cos k_y$
d_{xy} – wave	$\sin k_x \sin k_y$
p – wave	$a \sin k_x + b \sin k_y$
…	

Nambu-Gorkov DCA for Superconducting State

Non-interacting part of Hamiltonian

$$H_0 = \sum_{\mathbf{k}} \Psi^\dagger_{\mathbf{k}}[\epsilon_{\mathbf{k}}\sigma_3 - \eta'(\mathbf{k})\sigma_1 + \eta''(\mathbf{k})\sigma_2]\Psi_{\mathbf{k}}$$

Pauli spin matrices

$$\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Green's function in SC state

$$\mathbf{G}(\mathbf{k}, i\omega_n) = [i\omega_n\sigma_0 - (\varepsilon_{\mathbf{k}} - \mu)\sigma_3 - \eta'(\mathbf{k})\sigma_1 - \eta''(\mathbf{k})\sigma_2 - \boldsymbol{\Sigma}_c(\mathbf{K}, i\omega_n)]^{-1}$$

Cluster self-energy

$$\boldsymbol{\Sigma}_c(\mathbf{K}, i\omega_n) = \begin{pmatrix} \Sigma_c(\mathbf{K}, i\omega_n) & \phi_c(\mathbf{K}, i\omega_n) \\ \phi^*_c(\mathbf{K}, -i\omega_n) & -\Sigma^*_c(\mathbf{K}, i\omega_n) \end{pmatrix}$$

Nambu-Gorkov DCA for Superconducting State …

(1) Coarse-graining

$$\bar{\mathbf{G}}(\mathbf{K}, i\omega_n) = \frac{N_c}{N} \sum_{\mathbf{k} \in \mathscr{P}_\mathbf{K}} \mathbf{G}(\mathbf{k}, i\omega_n) = \begin{pmatrix} \bar{G}(\mathbf{K}, i\omega_n) & \bar{F}(\mathbf{K}, i\omega_n) \\ \bar{F}^*(\mathbf{K}, -i\omega_n) & -\bar{G}(\mathbf{K}, i\omega_n) \end{pmatrix}$$

$$\mathbf{G}(\mathbf{k}, i\omega_n) = [i\omega_n\sigma_0 - (\varepsilon_\mathbf{k} - \mu)\sigma_3 - \eta'(\mathbf{k})\sigma_1 - \eta''(\mathbf{k})\sigma_2 - \mathbf{\Sigma}_c(\mathbf{K}, i\omega_n)]^{-1}$$

(2) Cluster exclusion

$$\mathscr{G}_0(\mathbf{K}, i\omega_n) = \left[\bar{\mathbf{G}}^{-1}(\mathbf{K}, i\omega_n) + \mathbf{\Sigma}_c(\mathbf{K}, i\omega_n)\right]^{-1}$$

(3) Cluster problem solution

$$S[\Psi^*, \Psi] = -\int_0^\beta d\tau \int_0^\beta d\tau' \sum_{ij,\sigma} \Psi^*_{i\sigma}(\tau)\mathscr{G}_{0,ij,\sigma}(\tau - \tau')\Psi_{j\sigma}(\tau) + \frac{U}{2}\int_0^\beta d\tau \sum_i \left[\Psi^*_i(\tau)\sigma_3\Psi_i(\tau)\right]\left[\Psi^*_i(\tau)\sigma_3\Psi_i(\tau)\right]$$

$$\mathbf{G}_{c,ij,\sigma}(\tau - \tau') = \frac{1}{Z}\int \mathscr{D}[\Psi^*\Psi]\Psi_i(\tau)\Psi^*_j(\tau')e^{-S[\Psi^*,\Psi]}; Z = \int \mathscr{D}[\Psi^*\Psi]e^{-S[\Psi^*,\Psi]}$$

(4) New self-energy

$$\mathbf{\Sigma}_c(\mathbf{K}, i\omega_n) = \mathscr{G}_0^{-1}(\mathbf{K}, i\omega_n) - \mathbf{G}_c^{-1}(\mathbf{K}, i\omega_n)$$

Comments

Superconducting order parameter

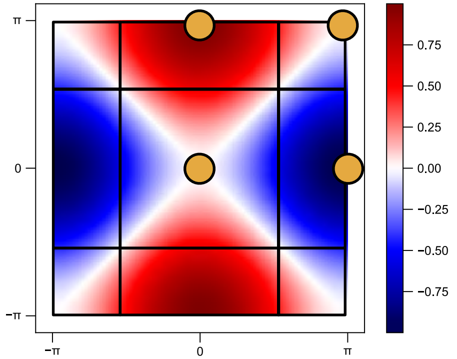
$$\bar{\Delta}(\mathbf{K}) = \frac{N_c}{N} \sum_{\mathbf{k} \in \mathscr{P}_{\mathbf{K}}} \langle c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow} \rangle = \bar{F}(\mathbf{K}, \tau = 0)$$

Study spontaneous symmetry breaking

- Initialize calculation with finite pair-field $\eta(\mathbf{k})$
- Switch off $\eta(\mathbf{k})$ after first (few) iterations
- Let system relax
- Calculate order parameter after convergence

Symmetry of superconducting state

- Given by $\boldsymbol{K}$-dependence of $\bar{\Delta}(\mathbf{K})$
- Possible symmetries constrained by cluster size and geometry



Symmetry	$\Delta_\mathbf{k}$	Nc=1 (DMFT)	Nc=4 (DCA)
s-wave	const.	✔	✔
Extended *s*-wave	$\cos k_x + \cos k_y$	✔	✔
$d_{x^2-y^2}$– wave	$\cos k_x - \cos k_y$	✘	✔
d_{xy} - wave	$\sin k_x \sin k_y$	✘	✘
p-wave	$a \sin k_x + b \sin k_y$	✘	✘
…			

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DCA Results for Superconducting State

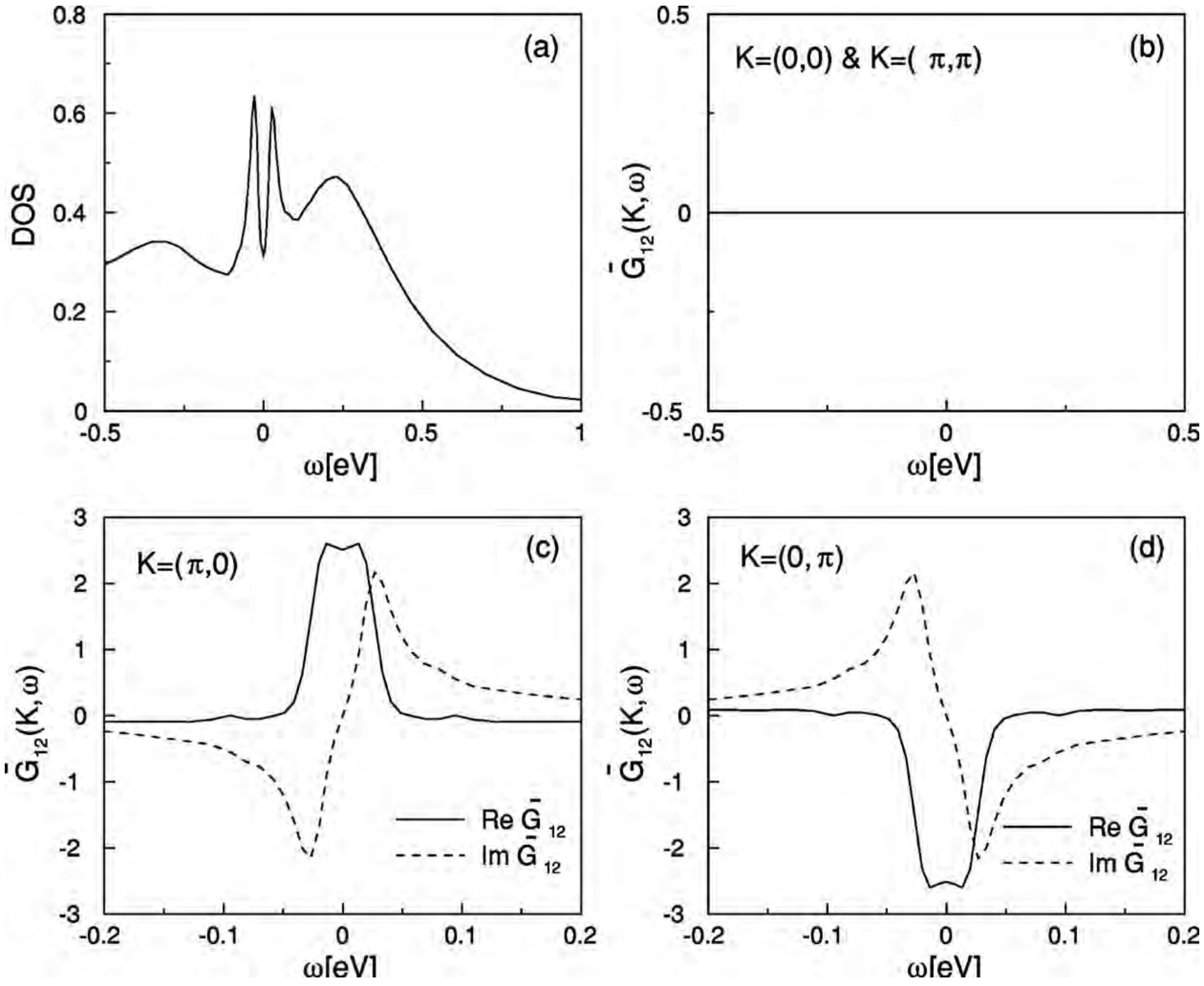
DCA (non-crossing approximation) results for SC state

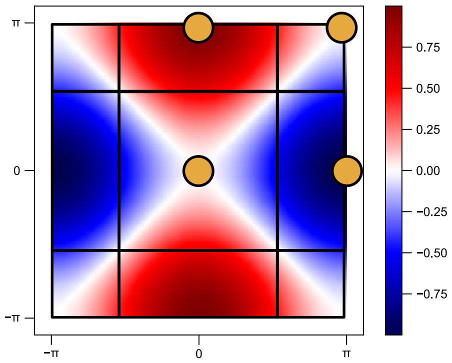
- Hubbard model; N_C=4, 2 x 2 cluster

$$U = 12t, \langle n \rangle = 0.81, T = 0.05t$$

- Anomalous Green's function is finite, vanishes for **K**=(0,0) and (π,π) and switches sign between **K**=(π,0) and (0,π)
  $\longrightarrow d_{x^2-y^2}$ – wave
- Superconducting gap is seen in density of states (DOS)

Maier et al., PRL 2000





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The Pair-Field Susceptibility

Definition

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

Pairing operator

$$\Delta_\alpha^\dagger = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} g_\alpha(\mathbf{k}) c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow}$$

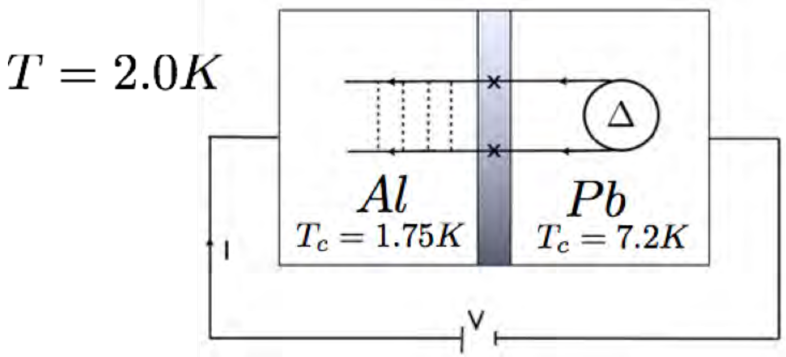
Form-factor (*d*-wave)

$$g_{d_{x^2-y^2}}(\mathbf{k}) = \cos k_x - \cos k_y$$

From Nambu-Gorkov DCA (DMFT)

$$P_\alpha = \left.\frac{d\Delta_\alpha(\eta_\alpha)}{d\eta_\alpha}\right|_{\eta_\alpha \to 0}$$

Tunnel junction between S and S' with $T_c(S) < T < T_c(S')$



Scalapino, PRL 24, 1052 (1970)
R. A. Ferrell, Low Temp. Phys. 1, 423 (1969)

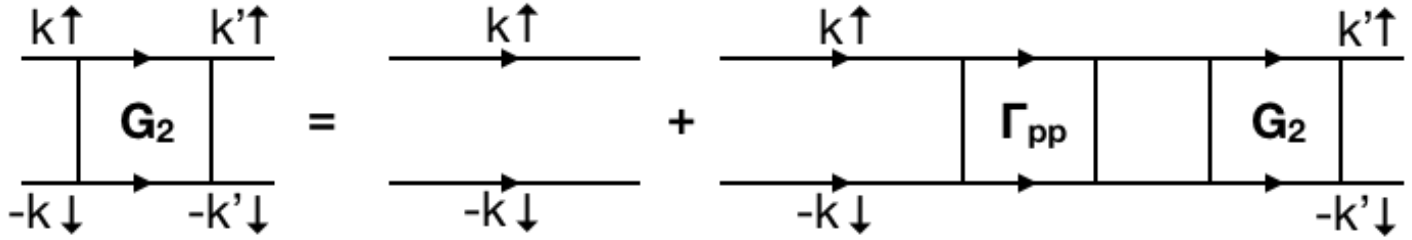
Direct Calculation of Response Function $P_\alpha(T) = \int_0^\beta d\tau \langle \Delta_\alpha(\tau)\Delta_\alpha^\dagger(0)\rangle$

From 4-point 2-particle Green's function

$$P_\alpha(T) = \frac{T^2}{N^2}\sum_{k,k'} g_\alpha(\mathbf{k}) G_{2,\uparrow\downarrow\downarrow\uparrow}(k,-k,-k',k') g_\alpha(\mathbf{k}')$$

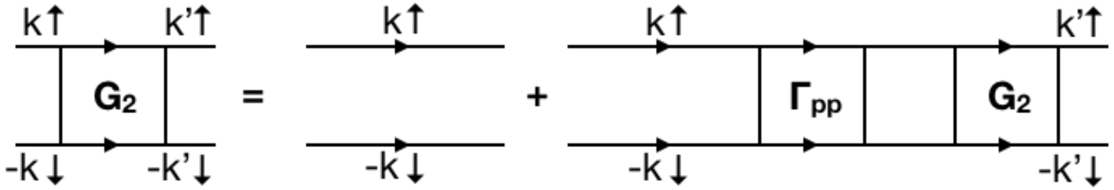
$$G_{2,\sigma_1\ldots\sigma_4}(x_1,x_2;x_3,x_4) = -\langle T_\tau c_{\sigma_1}(x_1) c_{\sigma_2}(x_2) c^\dagger_{\sigma_3}(x_3) c^\dagger_{\sigma_4}(x_4)\rangle \quad x_i = (\mathbf{X}_i, \tau_i)$$

$$G_{2,\uparrow\downarrow\downarrow\uparrow}(k,-k,-k',k') = G_\uparrow(k)G_\downarrow(-k)\delta_{k,k'} + \frac{T}{N}\sum_{k''} G_\uparrow(k)G_\downarrow(-k)\Gamma^{\mathrm{pp}}(k,-k,-k'',k'')G_{2,\uparrow\downarrow\downarrow\uparrow}(k'',-k'',-k',k')$$



DCA (DMFT) Approximation

Lattice 4-point correlation function



$$G_{2,\uparrow\downarrow\downarrow\uparrow}(k,-k,-k',k') = G_{\uparrow}(k)G_{\downarrow}(-k)\delta_{k,k'} + \frac{T}{N}\sum_{k''} G_{\uparrow}(k)G_{\downarrow}(-k)\Gamma^{\mathrm{pp}}(k,-k,-k'',k'')G_{2,\uparrow\downarrow\downarrow\uparrow}(k'',-k'',-k',k')$$

$$\Gamma^{\mathrm{pp}}(k,-k,-k',k') \approx \Gamma_c^{\mathrm{pp}}(K,-K,-K',K')$$

Cluster 4-point correlation function

$$G_{2c,\uparrow\downarrow\downarrow\uparrow}(K,-K,-K',K') = G_{c,\uparrow}(K)G_{c,\downarrow}(-K)\delta_{K,K'} + \frac{T}{N_c}\sum_{K''} G_{c,\uparrow}(K)G_{c,\downarrow}(-K)\Gamma_{c,pp}(K,-K,-K'',K'')G_{2c,\uparrow\downarrow\downarrow\uparrow}(K'',-K'',-K',K')$$

$$\longrightarrow\ P_\alpha(T) = \frac{T^2}{N_c^2}\sum_{K,K'} \bar{g}_\alpha(\mathbf{K})\bar{G}_{2,\uparrow\downarrow\downarrow\uparrow}(K,-K,-K',K')\bar{g}_\alpha(\mathbf{K}')$$

Bethe-Salpeter Eigenvalues And Eigenfunctions

Bethe-Salpeter equation (in matrix notation)

$$\bar{\mathbf{G}}_2 = [1 - \bar{\mathbf{G}}^0_{2,\uparrow\downarrow}\mathbf{\Gamma}^{\rm pp}_c]^{-1}\bar{\mathbf{G}}^0_{2,\uparrow\downarrow} = \bar{\mathbf{G}}^0_{2,\uparrow\downarrow}[1 - \mathbf{\Gamma}^{\rm pp}_c\bar{\mathbf{G}}^0_{2,\uparrow\downarrow}]^{-1}$$

"Pairing matrix" eigenvalues and eigenvectors

$$-\frac{T}{N_c}\sum_{K'}\Gamma_{c,pp}(K,K')\bar{G}^0_{2,\uparrow\downarrow}(K')\phi^R_\alpha(K') = \lambda_\alpha\phi^R_\alpha(K)$$

$$\longrightarrow \bar{G}_{2,\uparrow\downarrow\downarrow\uparrow}(K,K') = \bar{G}^0_{2,\uparrow\downarrow}(K)\sum_\alpha\frac{\phi^R_\alpha(K)\phi^L_\alpha(K')}{1-\lambda_\alpha}$$

Fully renormalized version of linearized BCS gap equation

$$-\frac{1}{N}\sum_{\mathbf{k}'}\frac{V(\mathbf{k},\mathbf{k}')\tanh\left(\frac{\beta}{2}E_{\mathbf{k}'}\right)\Delta(\mathbf{k}')}{2E_{\mathbf{k}'}} = \Delta(\mathbf{k}')$$

- Superconducting instability when leading eigenvalue $\lambda_\alpha = 1$
- K dependence of leading eigenvector $\Phi_\alpha(K)$ determines symmetry of superconducting state

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Superconductivity in the 2D attractive Hubbard model

$$\mathscr{H} = \sum_{ij,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}\,; \quad U < 0$$

DCA for Attractive Hubbard Model: General Considerations

Attractive Hubbard model

- $U < 0 \rightarrow$ local *s*-wave pairing interaction
- Toy model to study superconductivity
- No fermion sign problem in QMC!

General properties

- Finite *T* superconducting phase for $\langle n \rangle < 1$ with *s*-wave symmetry
- For $\langle n \rangle = 1$, degeneracy with charge density wave phase suppresses *SC* phase to T=0.

Mermin-Wagner theorem

- No finite-*T* long-range order in 2D due to breaking of continuous symmetry (U(1) gauge).

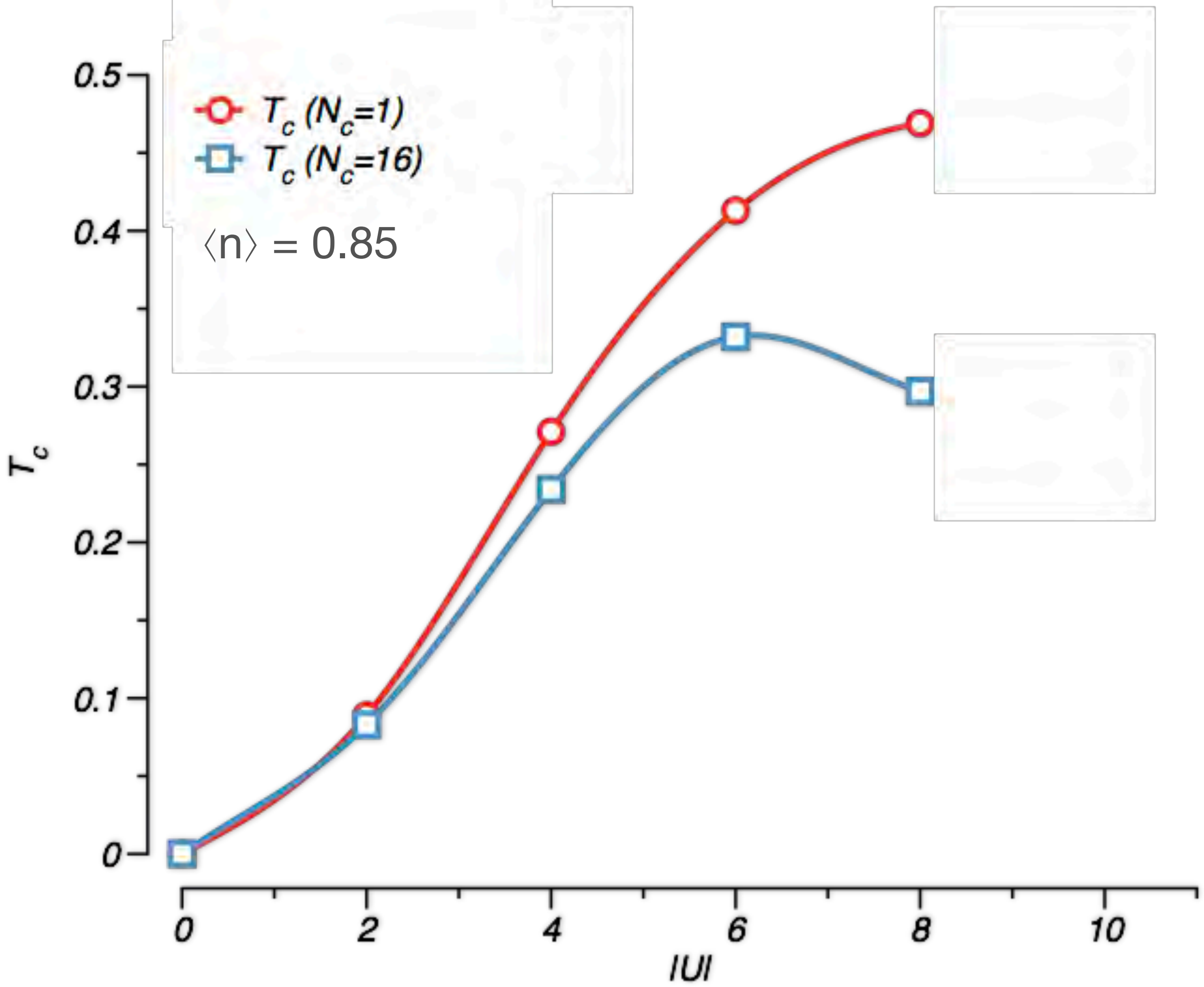
Kosterlitz-Thouless (KT) phase transition

- Superconducting correlations decay algebraically

DMFT & DCA

- Cut-off long-range correlations
- Do not obey Mermin-Wagner
- Mean-field behavior close to T_c
- KT behavior at higher *T*

Superconductivity in Attractive Hubbard Model: DMFT & DCA



Weak coupling (|*U*|< W)

- T_C rises with *U* due to pair-binding energy ~ *U*
- Expected BCS behavior

Strong coupling (|*U*|> W)

- T_C levels off in DMFT, falls in DCA
- BEC behavior: Tightly coupled pairs are not phase coherent
- DMFT only knows about temporal phase fluctuations
- DCA also describes spatial phase fluctuations

Superconductivity in Attractive Hubbard Model: DCA⁺

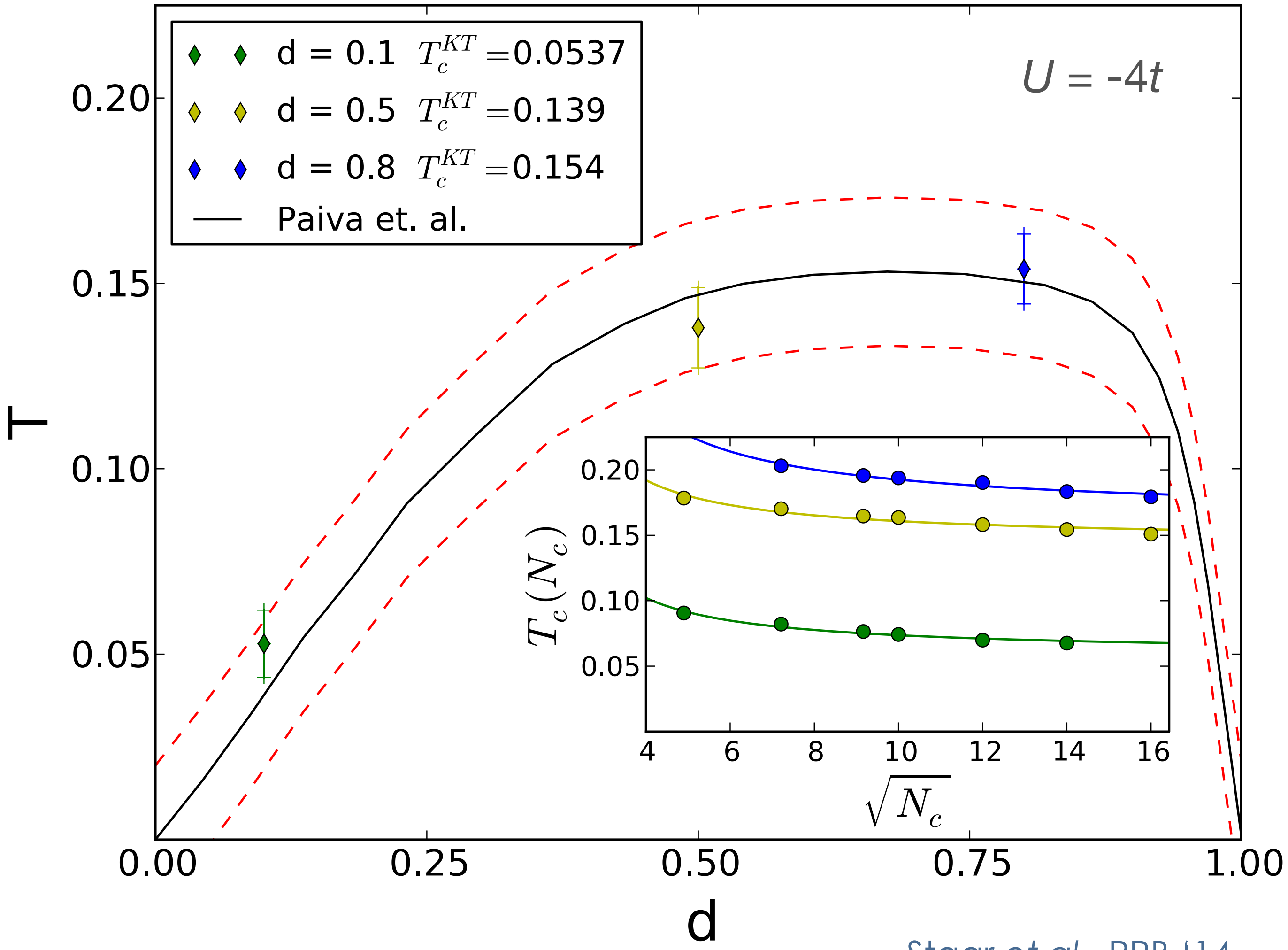
DCA finite size scaling

$$T_c(N_c) = T_{\mathrm{KT}} + \frac{A}{[B + \log(\sqrt{N_c})]^2}$$

- From $\xi(T) \sim e^{\frac{c}{\sqrt{T - T_{\mathrm{KT}}}}}$

  and $\xi(T_c(N_c)) = \sqrt{N_c}$

- DCA results agree well with finite lattice QMC results (Paiva et al., PRB '04)



Staar *et al.*, PRB '14

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Superconductivity in the 2D repulsive Hubbard model

$$\mathscr{H} = \sum_{ij,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}\,; \quad U > 0$$

Superconductivity in 2D Repulsive Hubbard Model? … An Open Question

Relevant to cuprates

- P. Anderson, Science ’87

Weak coupling theory

- Kohn & Luttinger, PRL ’65
- Scalapino et al., PRB ’86
- Zanchi & Schulz, PRB ’96
- Salmhofer, Comm. Math. Phys. ’98
- Halboth & Metzner, PRB ’00
- Honerkamp et al., PRB ‘01
- Binz et al., Ann. Phys. ’03
- Reiss et al., PRB ’07
- Zhai et al., PRB ’09
- Raghu et al., PRB ’10
- …

Intermediate/realistic coupling

- Quantum Monte Carlo ??
- Density matrix renormalization group ??
- DCA: Yes !

Pairing symmetry

- *s-wave* energetically unfavorable due to on-site Hubbard U
- $d_{x^2-y^2}$ – wave possible

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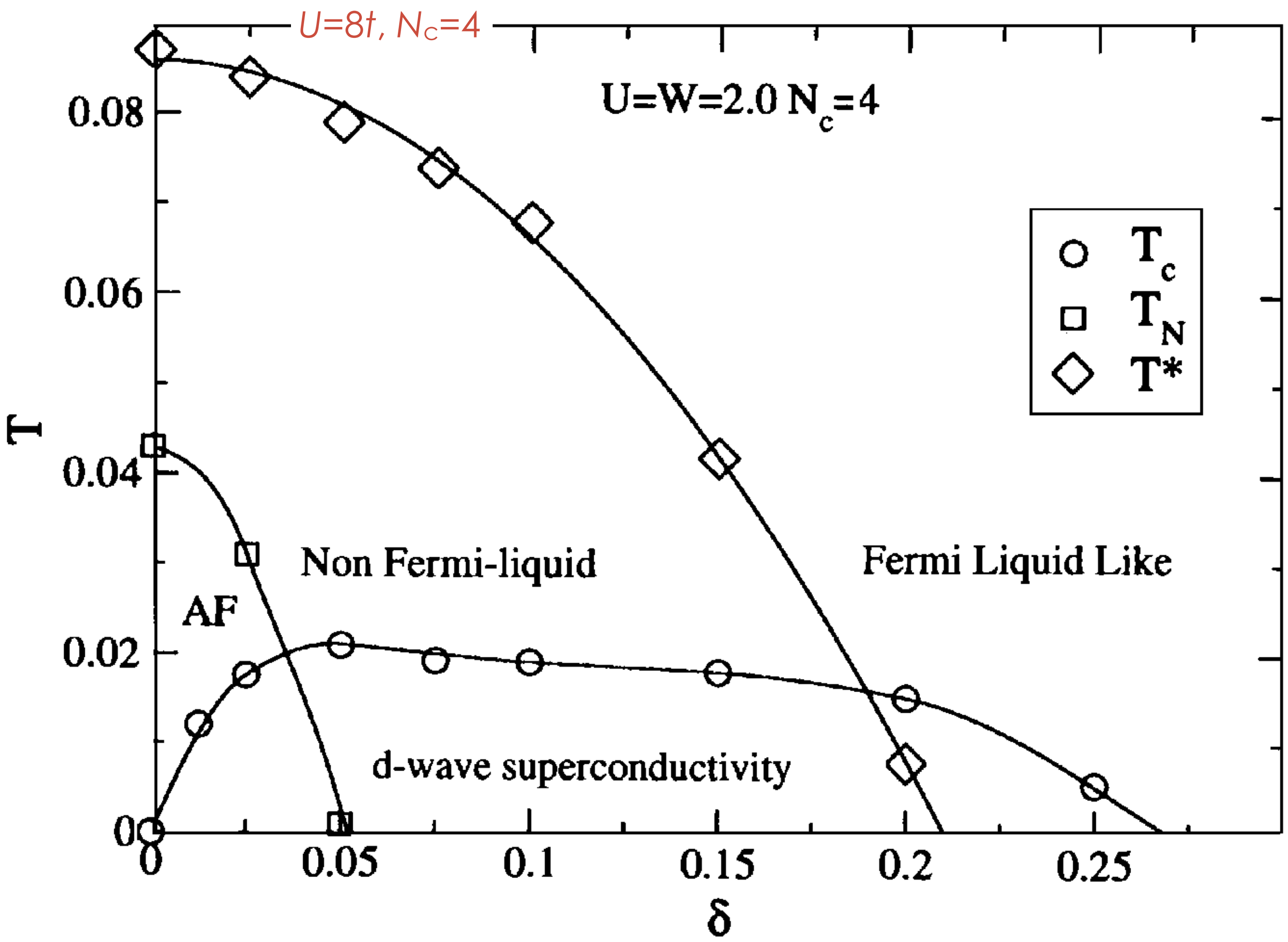
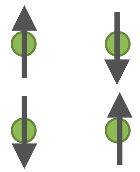
DCA Temperature Doping Phase Diagram: 2×2 Cluster



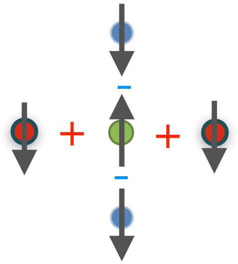
Jarrell *et al.*, EPL '01

DCA (QMC) for $U=8t$

- Antiferromagnet for $\langle n \rangle=1$



- d_{x2-y2} – wave superconducting for $\langle n \rangle < 1$



- Pseudogap below T^*

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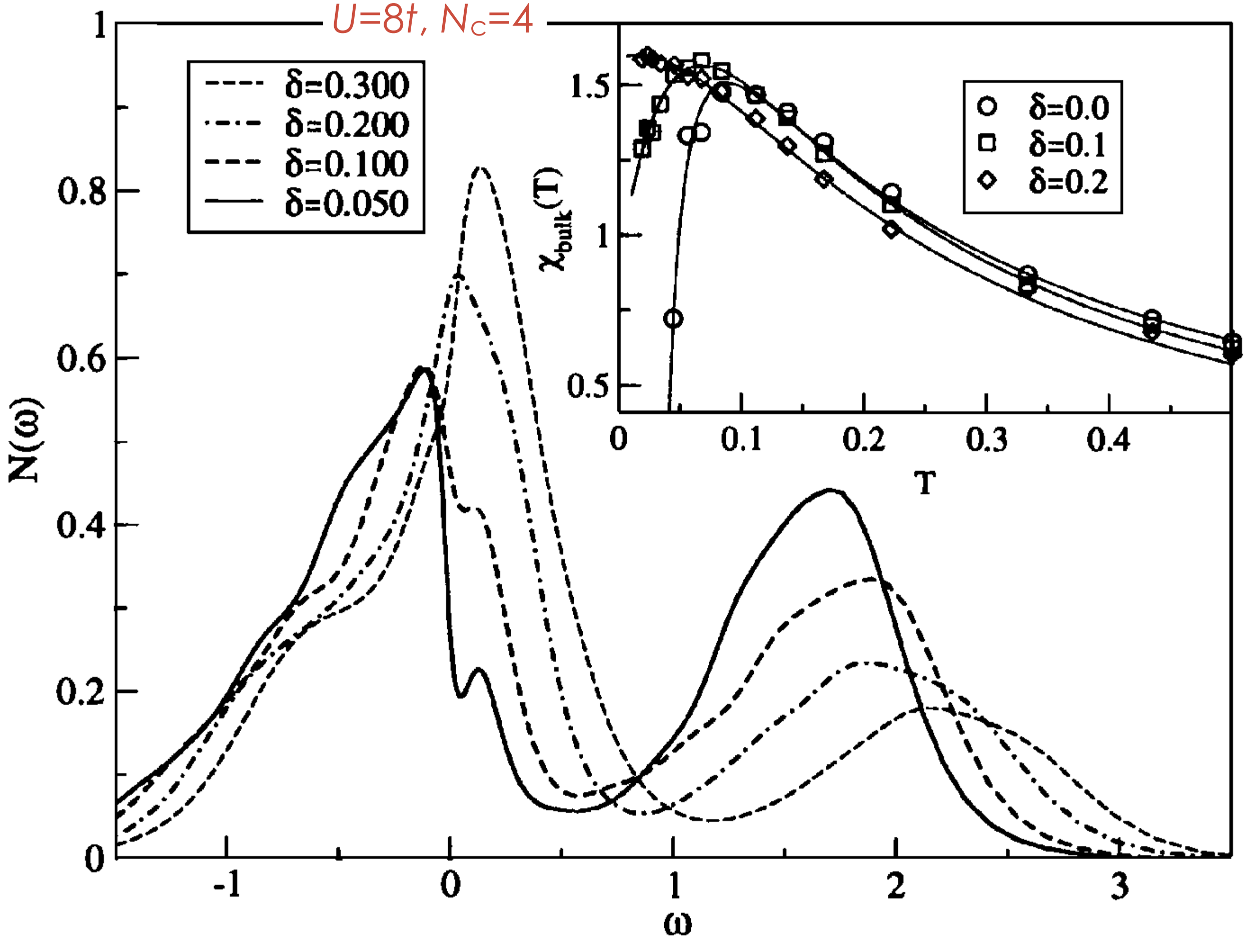
Pseudogap in 2D Hubbard Model

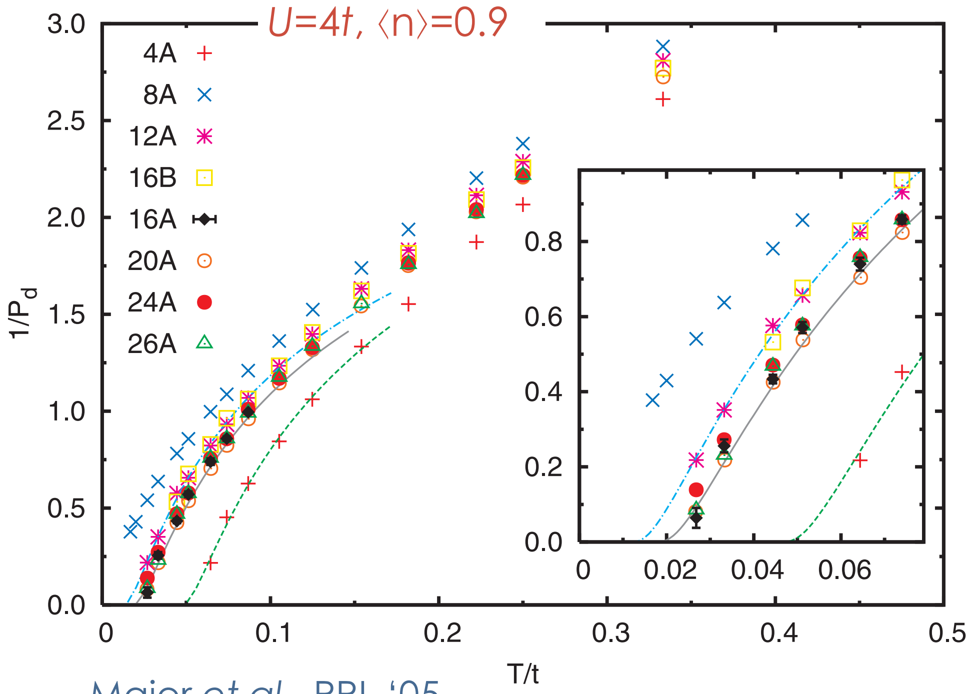
Pseudogap

- Bulk magnetic susceptibility exhibits downturn for $T < T^*$
- Partial suppression of density of states $N(\omega=0)$
- Demonstrates that superconductivity, just like in the cuprates, emerges out of an exotic, strange metal, non-Fermi liquid state

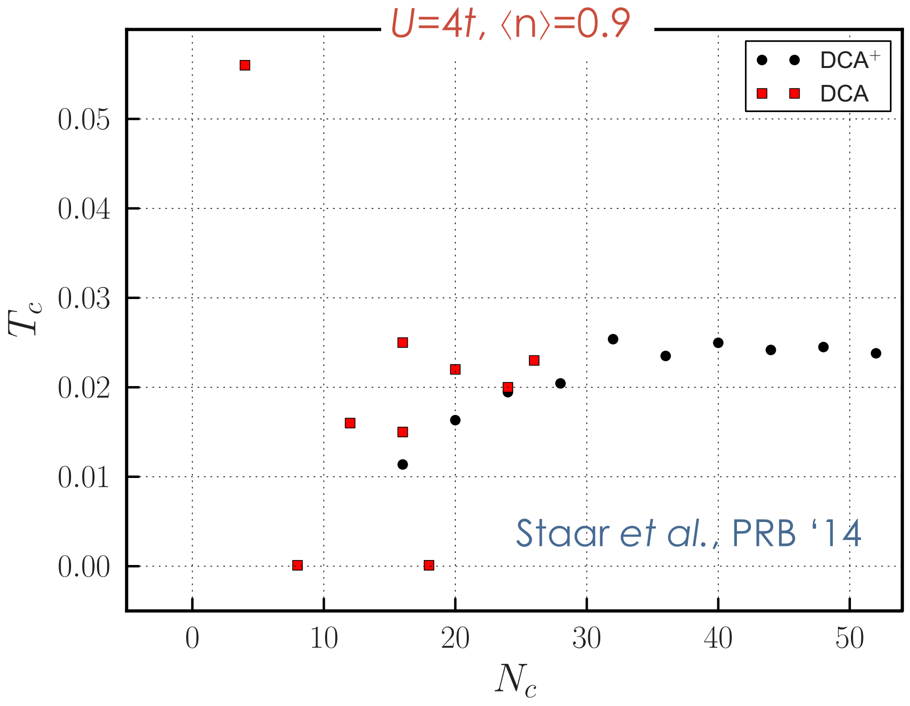


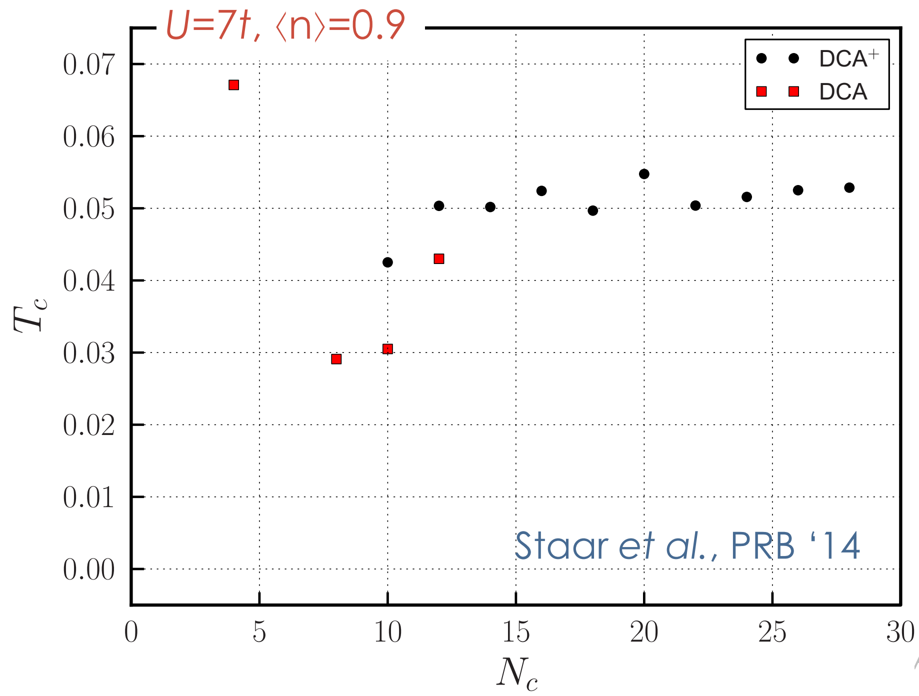
Jarrell *et al.*, EPL '01

Superconductivity in Exact ($N_c = \infty$) Limit?



Maier *et al.*, PRL '05





DCA$^{(+)}$ predicts **$d_{x2\text{-}y2}$–wave superconductivity** with **T_c ~ 0.05t** for realistic parameters (U=7t)

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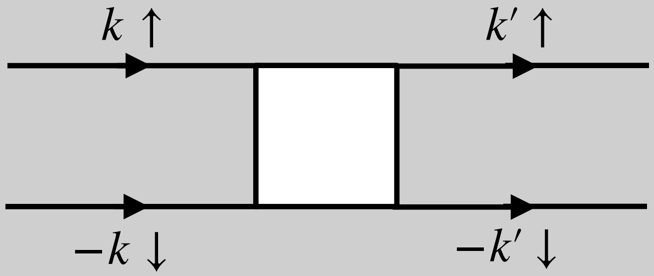
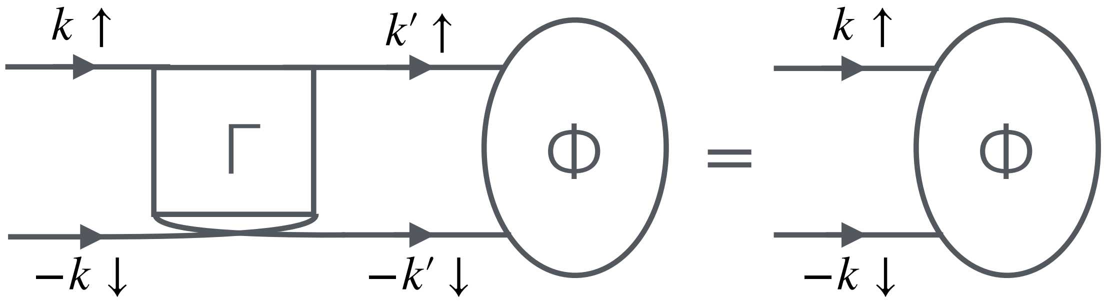
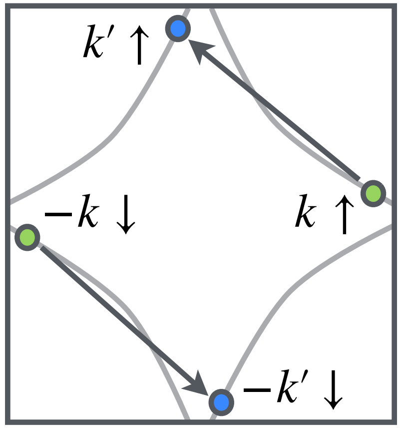
The Pairing Mechanism



Pairing Interaction: Irreducible Particle-Particle Vertex and Bethe-Salpeter Equation



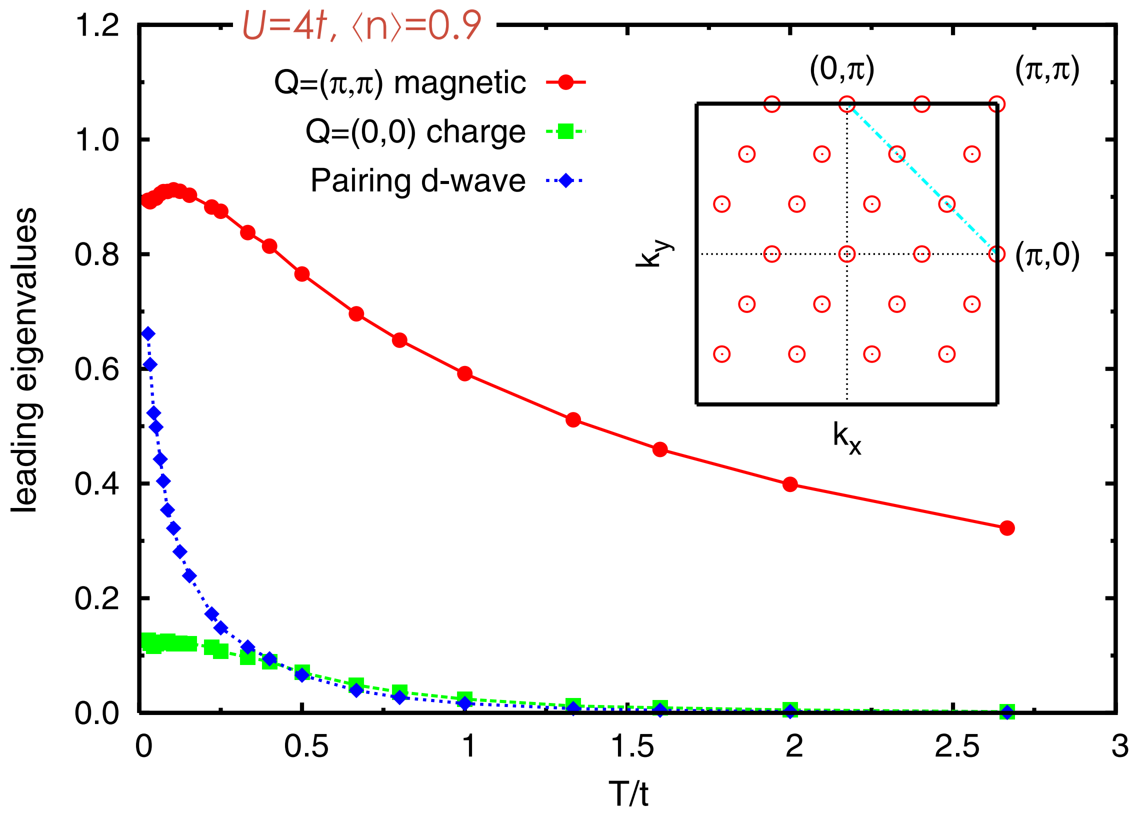


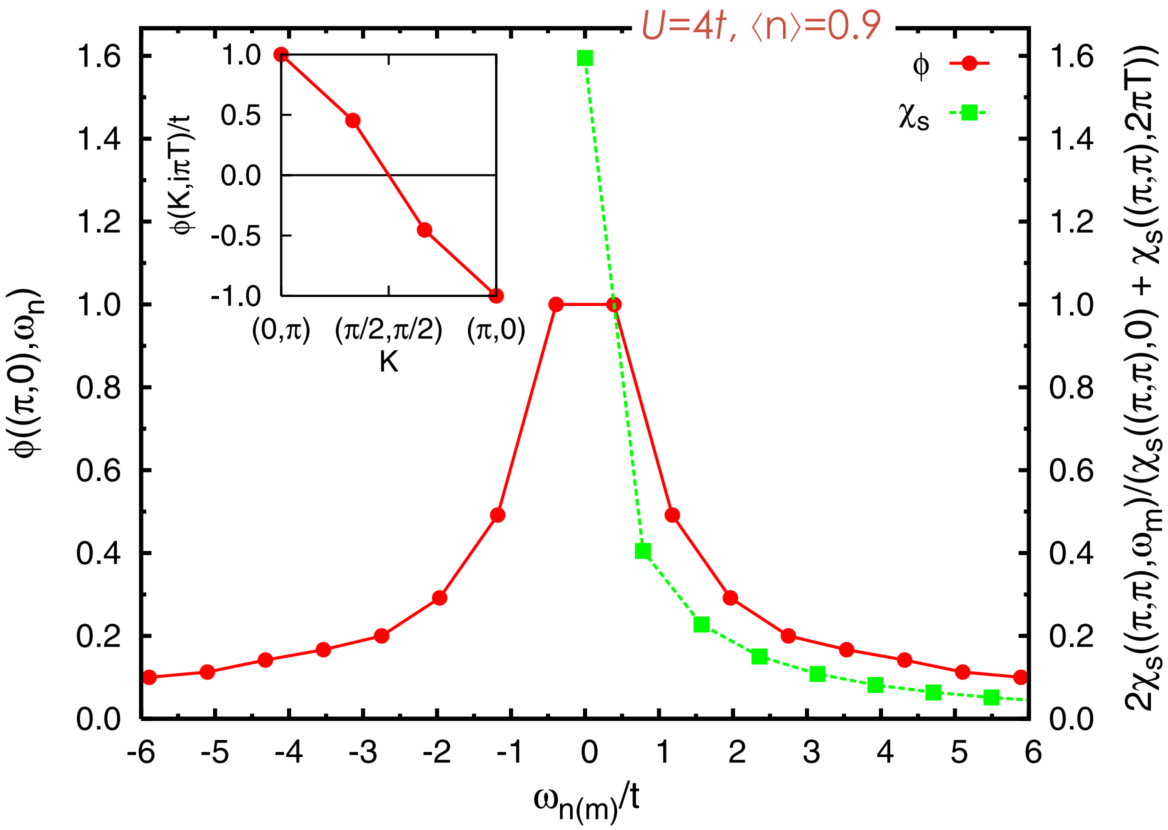
$$-\frac{T}{N_c}\sum_{K'}\Gamma_{c,pp}(K,K')\bar{G}^0_{2,\uparrow\downarrow}(K')\phi^R_\alpha(K') = \lambda_\alpha \phi^R_\alpha(K)$$

Compute exactly with DCA (QMC)

Leading Eigenvalues and -Vectors

Maier *et al.*, PRB '06





Leading correlations in **particle-hole**, spin S=1, **antiferromagnetic** (Q=(π,π)) and **particle-particle Q=0 pairing** channels. Leading pairing eigenvector has ***d*$_{x2\text{-}y2}$ – wave** momentum structure and reflects **spin fluctuation** frequency dependence.

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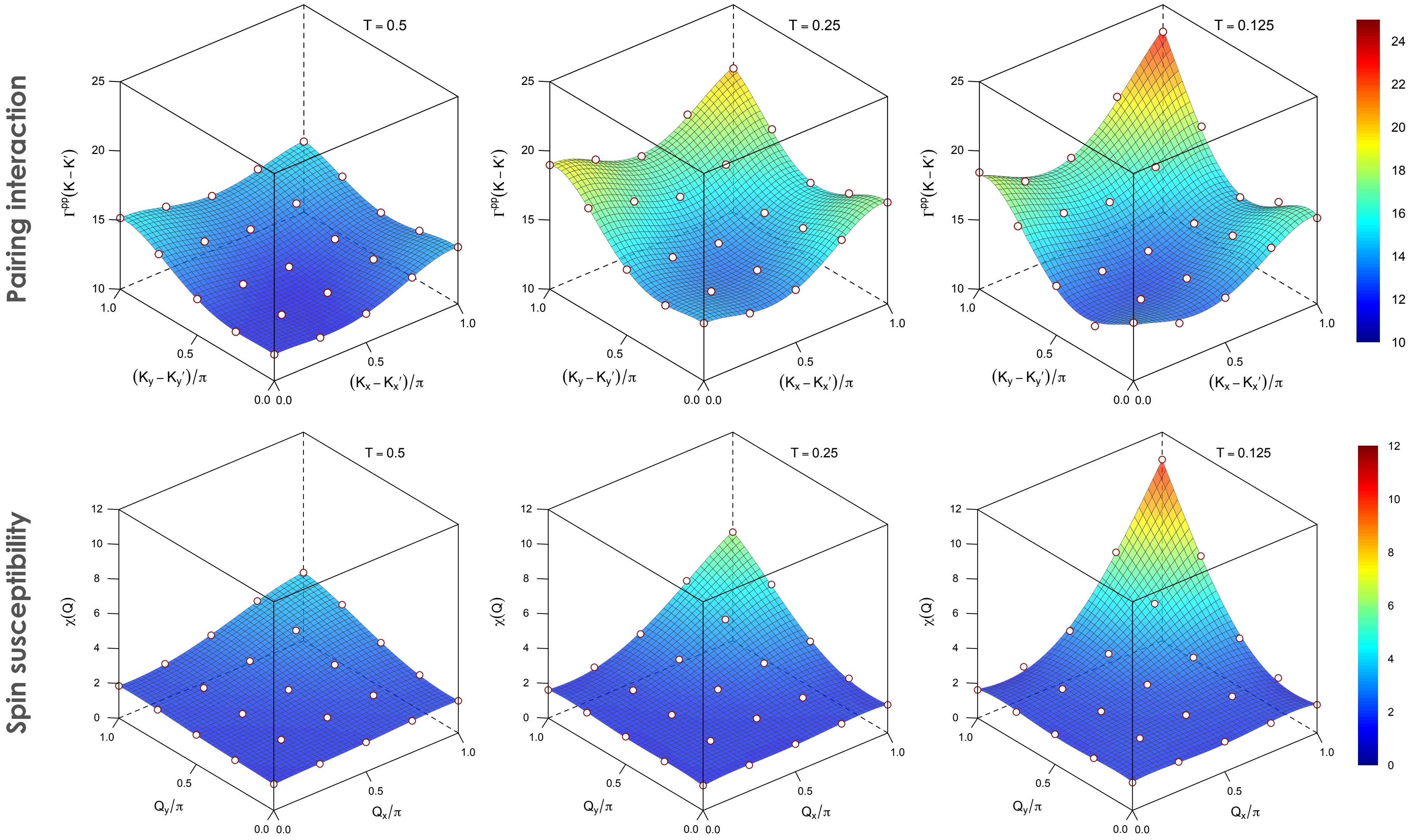
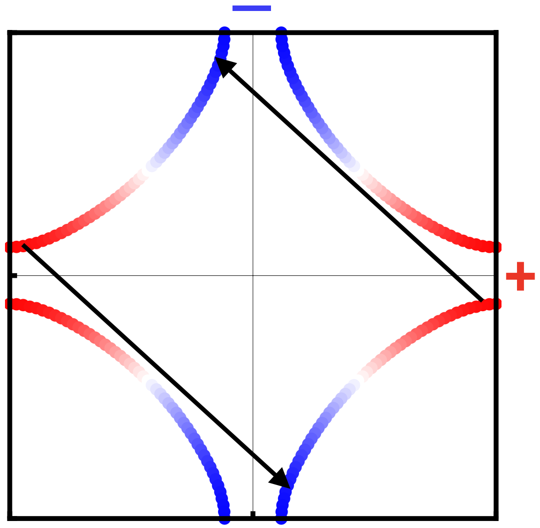
Momentum Structure of Pairing Interaction



How Does a Repulsive Interaction Give Pairing?

Momentum space

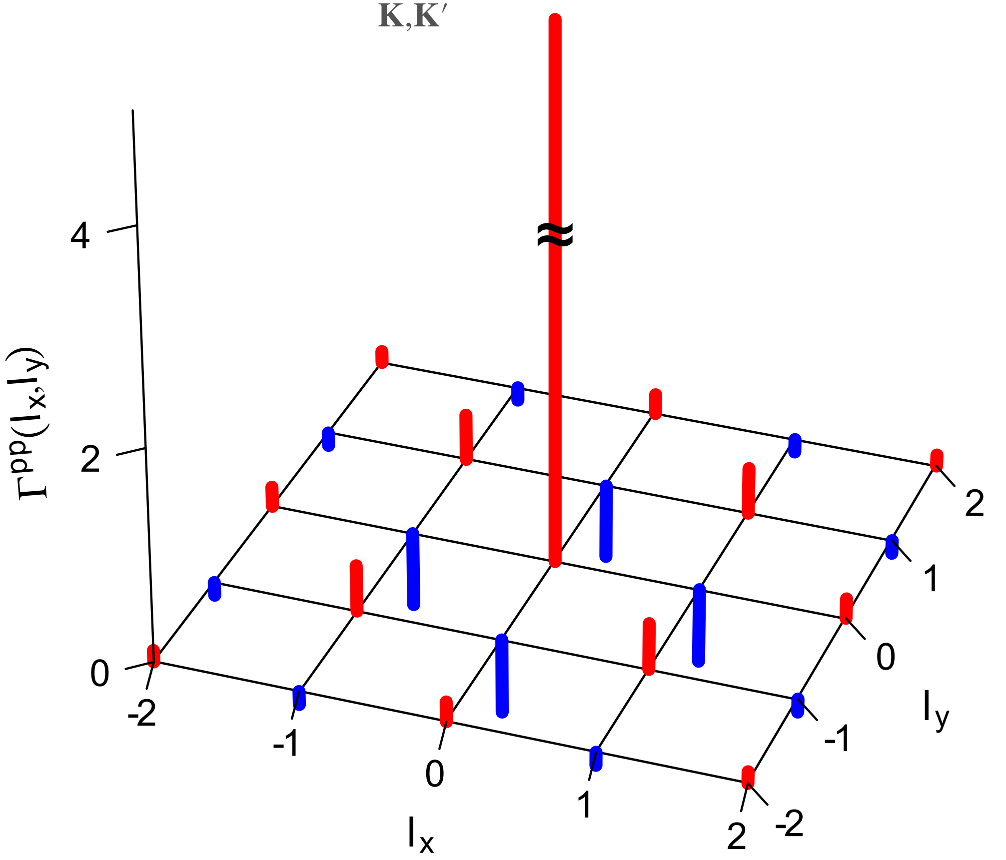
$$-\frac{T}{N_c}\sum_{K'}\Gamma_{c,pp}(K,K')\bar{G}^0_{2,\uparrow\downarrow}(K')\phi^R_\alpha(K')=\lambda_\alpha\phi^R_\alpha(K)$$



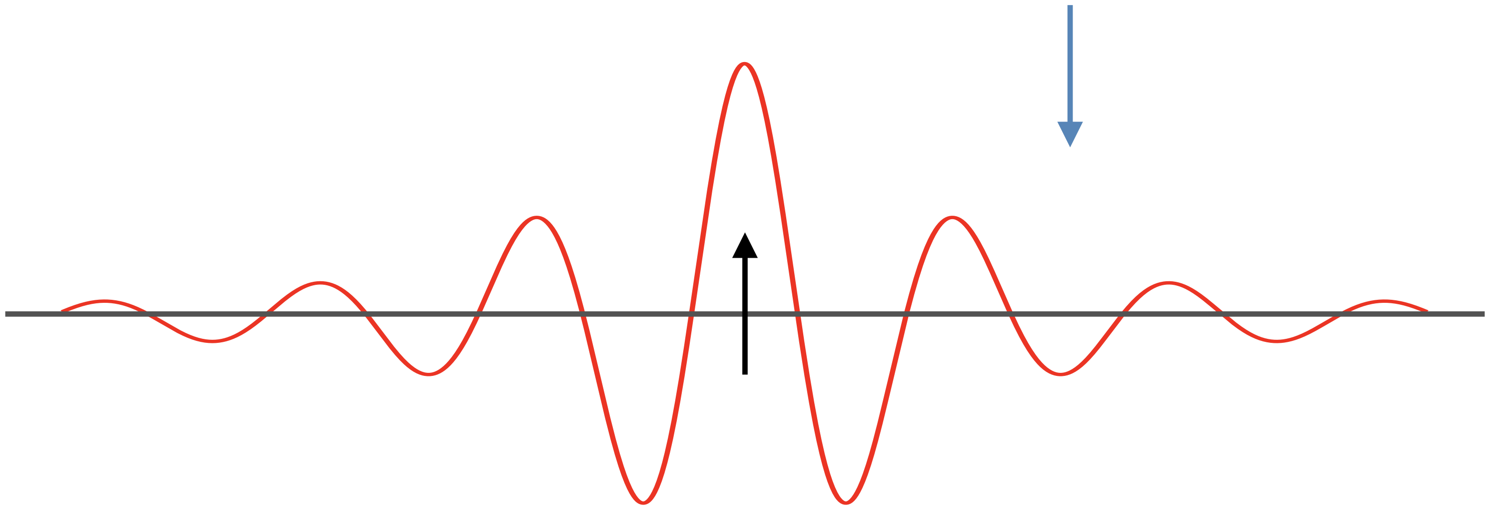
Momentum structure of pairing interaction gives rise to **attractive interaction** for **nearest-neighbor $d_{x2\text{-}y2}$ – wave** pairs

Real space

$$\Gamma^{pp}(\ell_x,\ell_y)=\sum_{\mathbf{K},\mathbf{K}'}e^{i\mathbf{K}\ell}\Gamma^{pp}(\mathbf{K},\mathbf{K}')e^{i\mathbf{K}'\ell}$$



Spin-Fluctuation Pairing Interaction



$$\Gamma^{\rm pp}(\mathbf{k}, \omega_n, \mathbf{k}', \omega_{n'}) \approx \frac{3}{2}\bar{U}^2\chi_s(\mathbf{k}-\mathbf{k}', \omega_n - \omega_{n'})$$

Origin of Dome-Shaped T_c vs. Doping

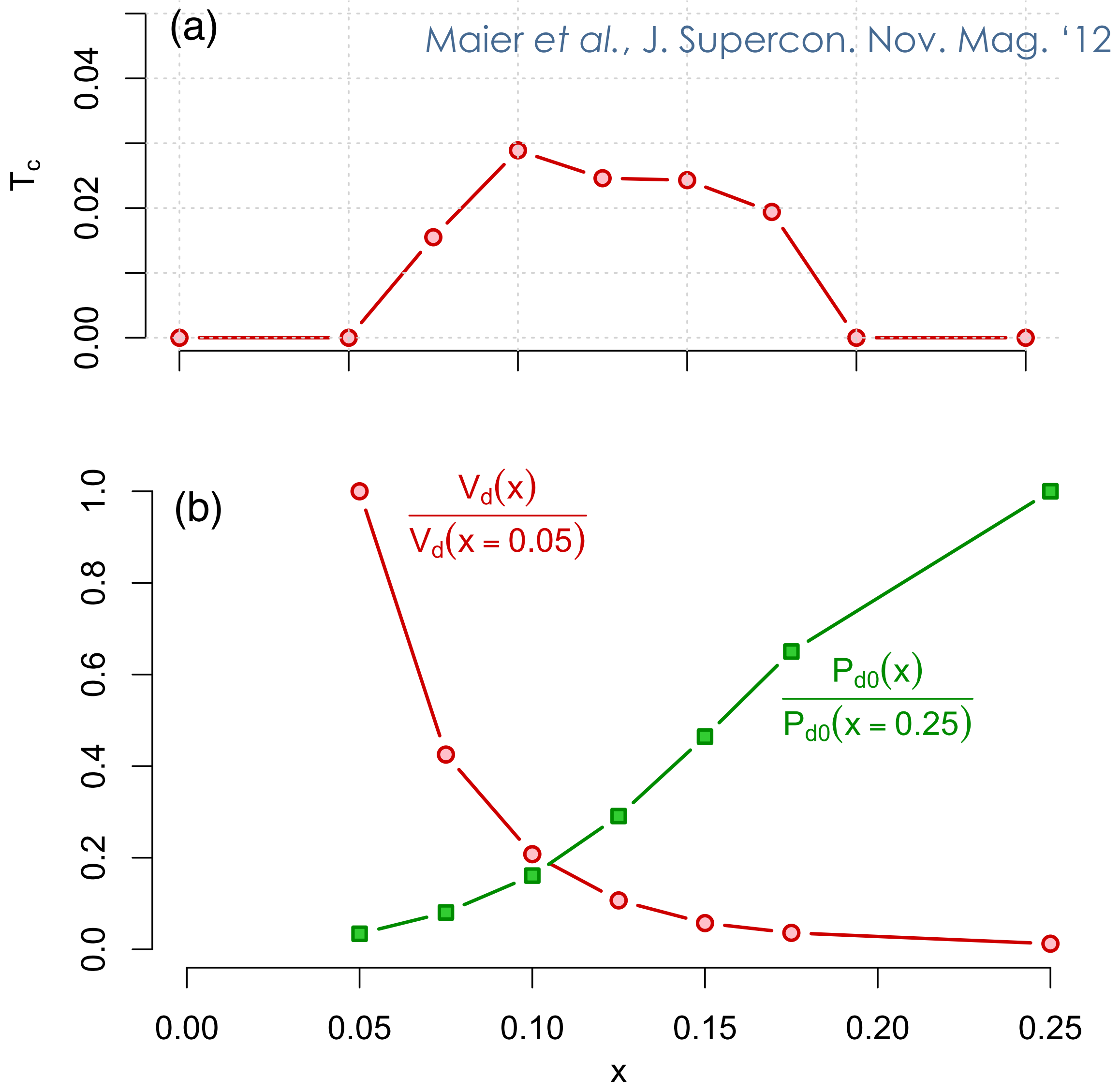
Separable approximation

$$\Gamma^{pp}(K,K') \approx -V_d\phi_d(K)\phi_d(K')$$

$$\rightarrow V_d(T)P_{d,0}(T) \approx \lambda_d$$

$$P_{d,0}(T) = T/N_c \sum_K \phi_d^2(K)\bar{G}^0_{2,\uparrow\downarrow}(K)$$

Opposite trends in doping dependence of $\boldsymbol{V_d}$ and $\boldsymbol{P_{d,0}}$ gives rise to **dome-shaped $\boldsymbol{T_c}$(x)**



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Extended Hubbard model

$$\mathscr{H} = \sum_{ij,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + V \sum_{\langle ij \rangle,\sigma\sigma'} n_{i\sigma} n_{j\sigma'}$$

Pairing and Retardation

Conventional electron-phonon superconductors

- Retardation is essential to overcome local Coulomb repulsion for s-wave pairs

Unconventional d-wave superconductors

- Local Coulomb repulsion is overcome by d-wave structure of pair wave function

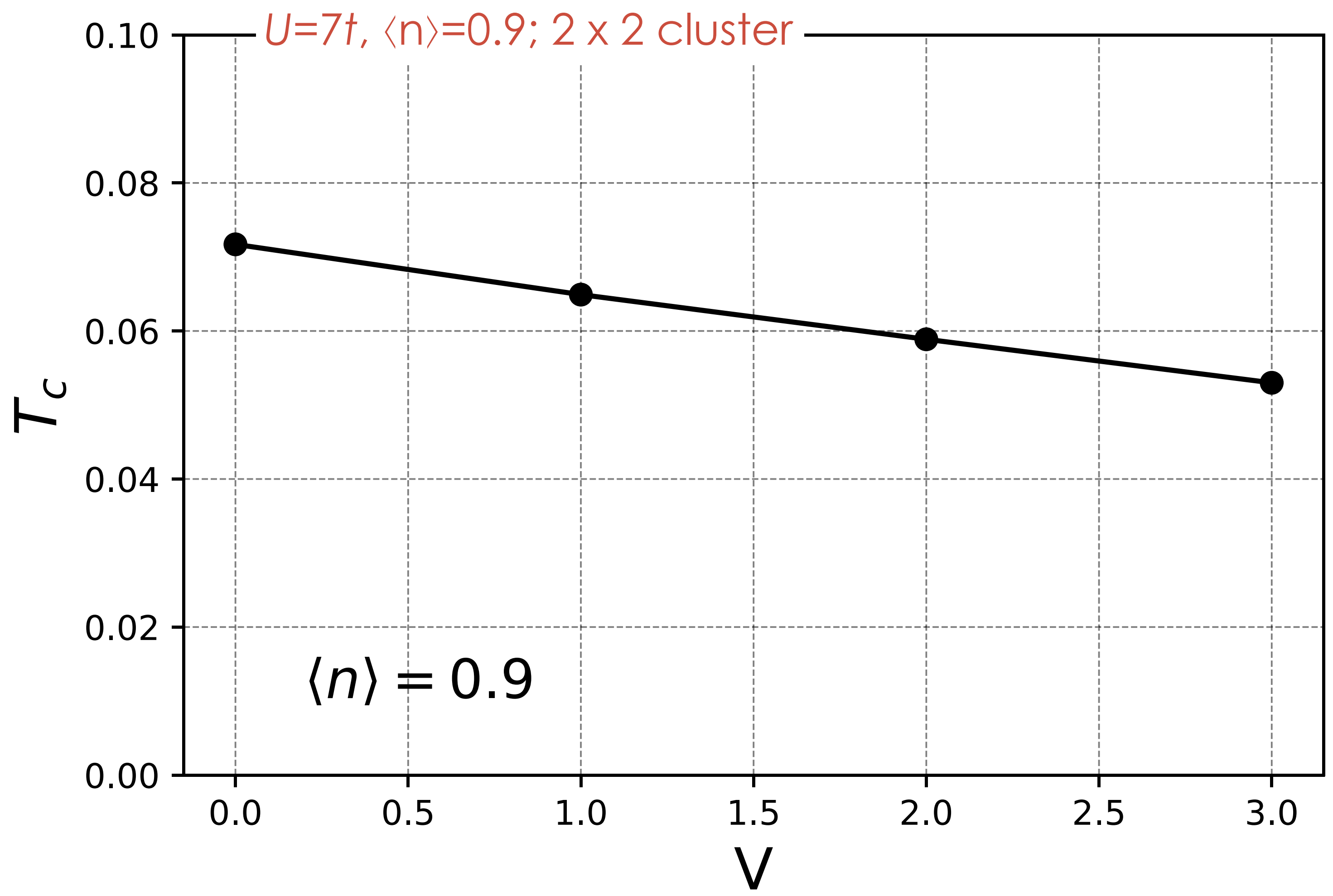
Extended Hubbard model

- Coulomb interaction in real materials not completely screened to local *U* → additional nearest neighbor *V* Coulomb repulsion

$$\mathscr{H} = \sum_{ij,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + V \sum_{\langle ij \rangle, \sigma\sigma'} n_{i\sigma} n_{j\sigma'}$$

- *V* is repulsive for nearest neighbor *d*-wave pairs
- Role of retardation?

DCA (QMC): T_c versus V



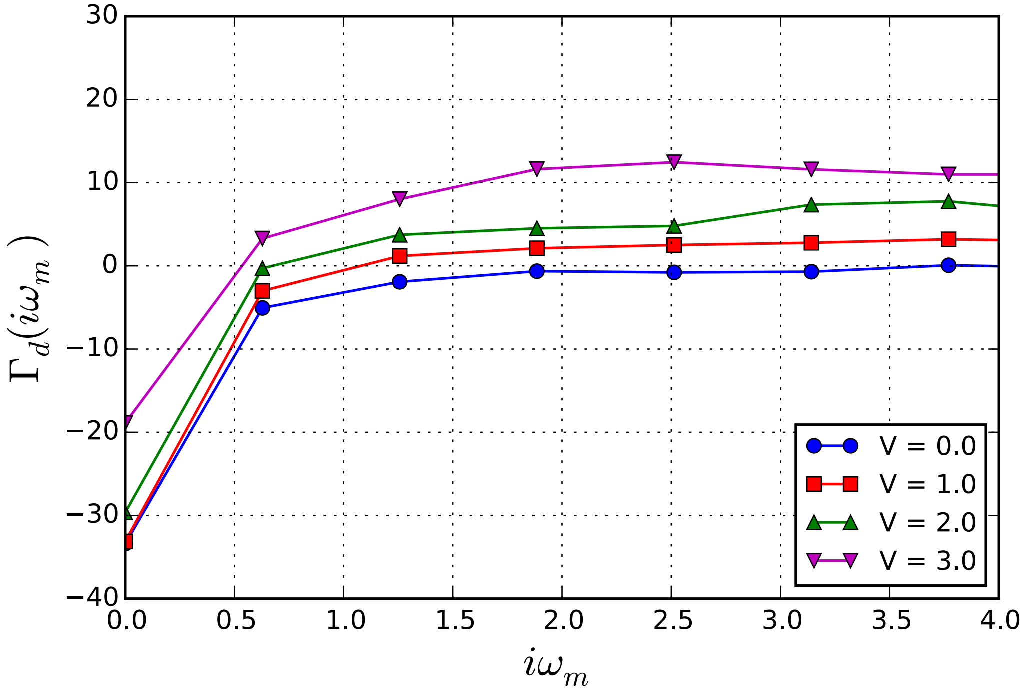
T_c **reduced by** ***V***, but rather **modestly**

Jiang *et al.*, PRB '18

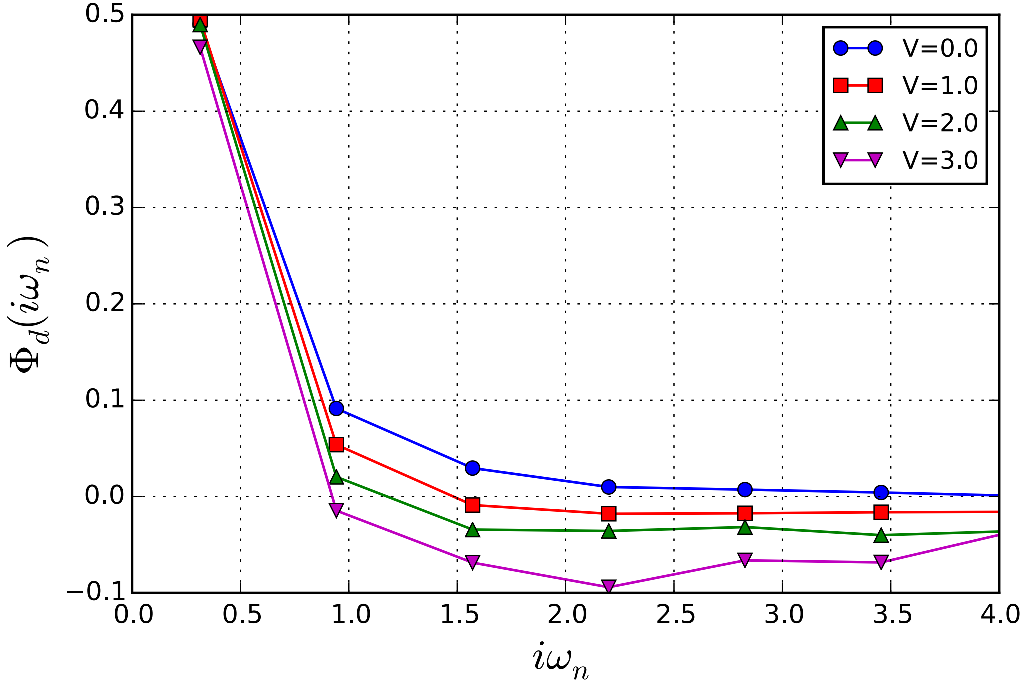
Role of Retardation

Jiang *et al.*, PRB '18

$$\Gamma_d(\omega_m = \omega_n - \omega_{n'}) = \frac{\sum_{\mathbf{K},\mathbf{K}'} g_d(\mathbf{K})\Gamma^{\mathrm{pp}}(\mathbf{K},\omega_n,\mathbf{K}',\omega_{n'})g_d(\mathbf{K}')}{\sum_{\mathbf{K}} g_d^2(\mathbf{K})}$$



d-wave eigenvector



D-wave pairing interaction is **attractive** at **low frequencies** and turns **repulsive** at **high frequencies** due to ***V***. **Sign change in** frequency dependence of ***d*-wave eigenvector** (gap function) **reduces repulsive effect of *V***.

Conclusions

- **DCA** (and DMFT) provide an **ideal framework** to study **superconductivity** in **strongly correlated quantum materials**, in the symmetry broken phase and from the normal state.

- **DCA** finds a ***d*-wave superconducting phase** in the **doped 2D Hubbard model** with **T_c ~ 0.05*t*** for realistic parameters, in addition to antiferromagnetic and pseudogap behavior.

- **DCA** calculations show that the **pairing interaction** increases with increasing momentum transfer and decreases when the energy transfer exceeds a scale associated with the **antiferromagnetic spin fluctuations**.

- This **retardation** reduces the repulsive effect of a nearest neighbor Coulomb repulsion in the extended Hubbard model.