Dynamical Mean Field and Dynamical Cluster Approximation Based Theory of Superconductivity

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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
**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

FIG. 1: Distribution of superconducting transition temperatures. The solid magenta bars represent the number of materials, \( N \), who's transition temperatures are tabulated in Fig. V.2 from Ref. [5], which includes over 500 superconducting materials known prior to 1979. Note that the numbers are shown on a log scale. We have added to the figure (the blue hatch bar) superconductors discovered since 1979 with transition temperatures in excess of 20K.

Since all the cuprate superconductors contain nearly square Cu-O planes, which are thought to be the central structure responsible for HTC, one might think of them all as one superconducting material. However, there are also differences between different cuprates, including the fact that some are n-type and some p-type, they have different numbers of proximate Cu-O planes, they can have different elements making up the charge reservoir layer, etc. There were 26 distinct crystal structures for cuprate superconductors tabulated in the 1994 monograph by Shaked et al. [6], so we have taken this as our definition of "distinct" materials. In each case, we have reported the highest transition temperature among different materials with the same crystal structure, restricting ourselves, however, to data at atmospheric pressure in bulk materials.

\( C_60 \) can be doped with different metal ions or mixtures of metal ions, but they all have more or less the same crystal structure and charge density, so we have counted this as one material (with a maximum \( T_c = 31 \) Ki in Rb\( _2 \)Cs\( _60 \)). One point is for BaKBiO (\( T_c = 31 \) K). We have also added one point for MgB\( _2 \) (\( T_c = 39 \) K). All of the organics and Na\( _0 \).3CoO\( _2 \)H\( 2 \)O have \( T_c \) less than our arbitrary cutoff, and so have been excluded.

Lurk in every third new material. At the crudest level, the dominant interaction between electrons is the strongly repulsive Coulomb interaction – for electrons to pair at all must involve subtle many-body effects which will therefore tend to be rather delicate. In BCS theory, it is the fact that the Coulomb interaction, \( \mu \), is well screened (short-ranged), and that the phonon-induced attraction, \( \lambda \), is highly retarded, that combines to make an effective attraction, \( \lambda_{eff} = \lambda - \mu \star \), between electrons at low energy. (This important point is stressed, for instance, in the classic Kivelson & Fradkin '05)

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

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

Barišić et al., Nat. Phys. ‘13

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

Keimer et al., Nature ‘15

Kivelson & Yao, Nat. Mat. ‘08
Cuprates: Electronic Structure & Hubbard Model

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

Anderson, Science ’87

Hashimoto et al., Nat. Phys. ’14
DMFT and Dynamic Cluster Approximation (DCA)
Preliminary Remarks

Thermodynamic Green’s function

\[ G_{ij,\sigma} = - \langle T_\tau c_{i\sigma} (\tau)c_{j\sigma}^\dagger \rangle \]

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

\[ G_{\sigma}(k, i\omega_n) \equiv \langle \langle c_{k,\sigma}; c_{k,\sigma}^\dagger \rangle \rangle_{i\omega_n} = \frac{1}{N} \sum_{ij} e^{ik(r_i-r_j)} G_{ij,\sigma}(i\omega_n) \]

Non-interacting \((U=0)\) Green’s function

\[ G_0(k, i\omega_n) = \frac{1}{i\omega_n + \mu - \varepsilon_k}; \quad \varepsilon_k = -2t(\cos k_x + \cos k_y) \]

Interacting Green’s function

\[ G(k, i\omega_n) = \frac{1}{G_0^{-1}(k, i\omega_n) - \Sigma(k, i\omega_n)} \]
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
\[ \Sigma(k, i\omega_n) \approx \Sigma_c(K, i\omega_n) \quad \text{(in DCA)} \]
\[ \Sigma(k, i\omega_n) \approx \Sigma_{ii}(i\omega_n) \quad \text{(in DMFT)} \]

Hettler et al., PRB '98
Maier et al., RMP '05
DCA (DMFT) Self-Consistency

(1) Coarse-graining
\[
\bar{G}(K, i\omega_n) = \frac{N_c}{N} \sum_{k \in \mathcal{P}_K} G(k, i\omega_n) = \frac{N_c}{N} \sum_{k \in \mathcal{P}_K} \frac{1}{i\omega_n - \epsilon_k + \mu - \Sigma_c(K, i\omega_n)}
\]

(2) Cluster exclusion
\[
\mathcal{G}_0(K, i\omega_n) = \left[ \bar{G}^{-1}(K, i\omega_n) + \Sigma_c(K, i\omega_n) \right]^{-1}
\]

(3) Cluster problem solution
\[
S[\phi^*, \phi] = -\int_0^\beta d\tau \int_0^\beta d\tau' \sum_{ij, \sigma} \phi_{i\sigma}^*(\tau) \mathcal{G}_{0,ij,\sigma}(\tau - \tau') \phi_{j\sigma}(\tau) + \int_0^\beta d\tau \sum_i U_{ii} \phi_{i\uparrow}^*(\tau) \phi_{i\uparrow}(\tau) \phi_{i\downarrow}^*(\tau) \phi_{i\downarrow}(\tau)
\]

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

(4) New self-energy
\[
\Sigma_c(K, i\omega_n) = \mathcal{G}_0^{-1}(K, i\omega_n) - G_c^{-1}(K, i\omega_n)
\]
Nambu-Gorkov Formalism for Superconducting State

Superconducting order parameter

\[ \Delta_k = \langle c_{k\uparrow} c_{-k\downarrow} \rangle \neq 0 \text{ for some } k \]

Anomalous Green's function

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

Nambu spinors

\[ \Psi_k^\dagger = \begin{pmatrix} c_{k\uparrow}^\dagger \\ c_{-k\downarrow}^\dagger \end{pmatrix} ; \Psi_k = \begin{pmatrix} c_{k\uparrow} \\ c_{-k\downarrow} \end{pmatrix} \]

Green's function matrix

\[
G(k, i\omega_n) = \langle \langle \Psi_k^\dagger \Psi_k \rangle \rangle_{i\omega_n} = \begin{pmatrix} G(k, i\omega_n) & F(k, i\omega_n) \\ F^*(k, -i\omega_n) & -G^*(k, i\omega_n) \end{pmatrix}
\]

<table>
<thead>
<tr>
<th>Symmetry</th>
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</tr>
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<tbody>
<tr>
<td>s-wave</td>
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<tr>
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<td>...</td>
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Nambu-Gorkov DCA for Superconducting State

Non-interacting part of Hamiltonian

\[ H_0 = \sum_k \Psi_k^\dagger [\epsilon_k \sigma_3 - \eta'(k) \sigma_1 + \eta''(k) \sigma_2] \Psi_k \]

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

\[ G(k, i\omega_n) = [i\omega_n \sigma_0 - (\epsilon_k - \mu) \sigma_3 - \eta'(k) \sigma_1 - \eta''(k) \sigma_2 - \Sigma_c(K, i\omega_n)]^{-1} \]

Cluster self-energy

\[ \Sigma_c(K, i\omega_n) = \begin{pmatrix} \Sigma_c(K, i\omega_n) & \phi_c(K, i\omega_n) \\ \phi_c^*(K, -i\omega_n) & -\Sigma^*_c(K, i\omega_n) \end{pmatrix} \]
Nambu-Gorkov DCA for Superconducting State...

(1) Coarse-graining

\[ \tilde{G}(K, i\omega_n) = \frac{N_c}{N} \sum_{k \in \mathcal{P}_K} G(k, i\omega_n) = \begin{pmatrix} \tilde{G}(K, i\omega_n) & F(K, i\omega_n) \\ \tilde{F}^*(K, -i\omega_n) & -\tilde{G}(K, i\omega_n) \end{pmatrix} \]

\[ G(k, i\omega_n) = \left[ i\omega_n \sigma_0 - (\varepsilon_k - \mu)\sigma_3 - \eta'(k)\sigma_1 - \eta''(k)\sigma_2 - \Sigma_c(K, i\omega_n) \right]^{-1} \]

(2) Cluster exclusion

\[ G_0(K, i\omega_n) = \left[ \tilde{G}^{-1}(K, i\omega_n) + \Sigma_c(K, i\omega_n) \right]^{-1} \]

(3) Cluster problem solution

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

\[ G_{c,ij,\sigma}(\tau - \tau') = \frac{1}{Z} \int \mathcal{D}[\Psi^*\Psi] \Psi_{i}(\tau) \Psi^*_{j}(\tau') e^{-S[\Psi^*,\Psi]} \]

(4) New self-energy

\[ \Sigma_c(K, i\omega_n) = G_0^{-1}(K, i\omega_n) - G_c^{-1}(K, i\omega_n) \]
Comments

Superconducting order parameter

\[ \tilde{\Delta}(\mathbf{K}) = \frac{N_c}{N} \sum_{\mathbf{k} \in \mathcal{P}_K} \langle c_{\mathbf{k} \uparrow} c_{-\mathbf{k} \downarrow} \rangle = \bar{F}(\mathbf{K}, \tau = 0) \]

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 \( \mathbf{K} \)-dependence of \( \tilde{\Delta}(\mathbf{K}) \)
- Possible symmetries constrained by cluster size and geometry

<table>
<thead>
<tr>
<th>Symmetry</th>
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<th>( N_c=1 ) (DMFT)</th>
<th>( N_c=4 ) (DCA)</th>
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DCA Results for Superconducting State

DCA (non-crossing approximation) results for SC state

- Hubbard model; \( N_c=4, 2 \times 2 \) cluster
  \[ U = 12t, \langle n \rangle = 0.81, T = 0.05t \]
- Anomalous Green’s function is finite, vanishes for \( \mathbf{K}=(0,0) \) and \((\pi,\pi)\) and switches sign between \( \mathbf{K}=(\pi,0) \) and \((0,\pi)\)
  \[ \rightarrow d_{x^2-y^2} – \text{wave} \]
- Superconducting gap is seen in density of states (DOS)

Maier et al., PRL 2000
The Pair-Field Susceptibility

Definition

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

Pairing operator

\[ \Delta_\alpha^\dagger = \frac{1}{\sqrt{N}} \sum_k g_\alpha(k)c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger \]

Form-factor \((d\text{-wave})\)

\[ g_{d_{2-\gamma^2}}(k) = \cos k_x - \cos k_y \]

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 \(T_c(S) < T < T_c(S')\)

\[ T = 2.0K \]

Scalapino, PRL 24, 1052 (1970)
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

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

\[ G_{2,\sigma_1...\sigma_4}(x_1, x_2; x_3, x_4) = - \langle T_{\tau} c_{\sigma_1}(x_1) c_{\sigma_2}(x_2) c_{\sigma_3}^{\dagger}(x_3) c_{\sigma_4}^{\dagger}(x_4) \rangle \quad x_i = (X_i, \tau_i) \]

\[ G_{2,\uparrow\downarrow\downarrow\downarrow}(k, -k, -k', k') = G_{\uparrow}(k) G_{\downarrow}(-k) \delta_{k,k'} + \frac{T}{N} \sum_{k''} G_{\uparrow}(k) G_{\downarrow}(-k) \Gamma_{pp}(k, -k, -k'', k'') G_{2,\uparrow\downarrow\downarrow\downarrow}(k'', -k'', -k', k') \]
DCA (DMFT) Approximation

Lattice 4-point correlation function

\[
G_{2,↑↓↓↑}(k, -k, -k', k') = G_1(k)G_4(-k)\delta_{k,k'} + \frac{T}{N} \sum_{k''} G_1(k)G_4(-k)\Gamma^{pp}(k, -k, -k'', k'')G_{2,↑↓↓↑}(k'', -k'', -k', k')
\]

Cluster 4-point correlation function

\[
G_{2c,↑↓↓↑}(K, -K, -K', K') = G_{c,1}(K)G_{c,4}(-K)\delta_{K,K'} + \frac{T}{N_c} \sum_{K''} G_{c,1}(K)G_{c,4}(-K)\Gamma^{pp}_{c,pp}(K, -K, -K'', K'')G_{2c,↑↓↓↑}(K'', -K'', -K', K')
\]

\[
\rightarrow P_\alpha(T) = \frac{T^2}{N_c^2} \sum_{K,K'} \bar{g}_\alpha(K)\bar{G}_{2,↑↓↓↑}(K, -K, -K', K')\bar{g}_\alpha(K')
\]
Bethe-Salpeter Eigenvalues And Eigenfunctions

Bethe-Salpeter equation (in matrix notation)

\[ \tilde{G}_2 = [1 - \tilde{G}_{2,\uparrow\downarrow}^0 \Gamma_{c,pp}^{\uparrow\downarrow}]^{-1} \tilde{G}_{2,\uparrow\downarrow}^0 = \tilde{G}_{2,\uparrow\downarrow}^0 [1 - \Gamma_{c,pp}^{\uparrow\downarrow} \tilde{G}_{2,\uparrow\downarrow}^0]^{-1} \]

"Pairing matrix" eigenvalues and eigenvectors

\[ -\frac{T}{N_c} \sum_{K'} \Gamma_{c,pp}(K, K') \tilde{G}_{2,\uparrow\downarrow}^0(K') \phi_{\alpha}^R(K') = \lambda_{\alpha} \phi_{\alpha}^R(K) \]

\[ \longrightarrow \tilde{G}_{2,\uparrow\downarrow\uparrow\downarrow}(K, K') = \tilde{G}_{2,\uparrow\downarrow}^0(K) \sum_{\alpha} \frac{\phi_{\alpha}^R(K) \phi_{\alpha}^L(K')}{1 - \lambda_{\alpha}} \]

Fully renormalized version of linearized BCS gap equation

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

- Superconducting instability when leading eigenvalue \( \lambda_{\alpha} = 1 \)
- \( K \) dependence of leading eigenvector \( \Phi_{\alpha}(K) \) determines symmetry of superconducting state
Superconductivity in the 2D attractive Hubbard model

\[ \mathcal{H} = \sum_{ij,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}; \quad U < 0 \]
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 $\sim U$
- 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

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

- From \( \xi(T) \sim e^{(T - T_{KT})} \)
- \( \xi(T_c(N_c)) = \sqrt{N_c} \)
- DCA results agree well with finite lattice QMC results (Paiva et al., PRB '04)

\[ U = -4t \]

\[ \begin{align*}
\text{d} & = 0.1 & T_c^{KT} &= 0.0537 \\
\text{d} & = 0.5 & T_c^{KT} &= 0.139 \\
\text{d} & = 0.8 & T_c^{KT} &= 0.154
\end{align*} \]

Staar et al., PRB '14
Superconductivity in the 2D repulsive Hubbard model

\[ \mathcal{H} = \sum_{ij,\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}; \quad U > 0 \]
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
- 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
The superconductivity persists to large doping, with the parts of the Fermi surface closest to $\pi$-wave pair-field susceptibility diverges at $d$. Fig. 5 – The temperature-doping phase diagram of the 2D Hubbard model calculated with QMC and corrections ($u_{\pi}$, $d_{\pi}$, $\delta$, $\kappa$) when multiple Hubbard planes are coupled together. The $e_{\text{t}}$ibility), therefore, the overlap of one, indicating that the fluctuations beyond DMFA which suppress the antiferromagnetism might happen from the paramagnetic state.

The phase diagram of the system is shown in fig. 5. We are determining the phase boundaries, with higher transition temperature is suppressed ($\delta^c \geq 0.2$). The phase diagram will stabilize the character of the phase diagram presented. For $J_0.2 \geq J_0.06$, the liquid behavior. For $d^c \geq 0.4, 0.5$, the pairing correlations are suppressed. In the 8A cluster where $zd \leq 4$, fluctuations are overestimated and the pair-field susceptibility as a function of temperature for different cluster sizes at 10% doping. Such work is currently in progress.

For $\delta^c = 4$, we include $T^c \sim 0.025$. This could be due to the lack of long-ranged dynamical correlations and the highest enhanced compared to the 8A cluster and the pair-field susceptibility as a function of temperature for different cluster sizes at 10% doping. A finite interplane coupling will also invalidate the Mermin-Wagner – Antiferromagnet for $\langle n \rangle = 1$

$- d_{x^2-y^2}$-wave superconducting for $\langle n \rangle < 1$

$- \text{Pseudogap below } T^*$

DCA (QMC) for $U=8t$

- Antiferromagnet for $\langle n \rangle = 1$
- $d_{x^2-y^2}$-wave superconducting for $\langle n \rangle < 1$
- Pseudogap below $T^*$

Jarrell et al., EPL ‘01
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

\[ U=8t, N_c=4 \]

Jarrell et al., EPL '01
Superconductivity in Exact \((N_c = \infty)\) Limit?

**DCA\(^{ (+) }\) predicts** \(d_{x^2-y^2}-\text{wave superconductivity} \) with \(T_c \sim 0.05t\) for realistic parameters (\(U=7t\))
The Pairing Mechanism
Pairing Interaction: Irreducible Particle-Particle Vertex and Bethe-Salpeter Equation

\[ -\frac{T}{N_c} \sum_{K'} \Gamma_{c,pp}(K, K') \bar{G}_2,\uparrow\downarrow(K') \phi_R^R(K') = \lambda_\alpha \phi_R^R(K) \]

Compute exactly with DCA (QMC)
Leading Eigenvalues and -Vectors

Leading correlations in particle-hole, spin $S=1$, antiferromagnetic ($Q=(\pi,\pi)$) and particle-particle Q=0 pairing channels. Leading pairing eigenvector has $d_{x^2-y^2}$ wave momentum structure and reflects spin fluctuation frequency dependence.

Maier et al., PRB '06
Momentum Structure of Pairing Interaction
How Does a Repulsive Interaction Give Pairing?

Momentum space

\[-\frac{T}{N_c} \sum_{K'} \Gamma_{c,pp}(K, K')\mathcal{G}^0_{2,1\downarrow}(K')\phi^R(K') = \lambda_\alpha \phi^R(K)\]

Momentum structure of pairing interaction gives rise to attractive interaction for nearest-neighbor $d_{x^2-y^2}$-wave pairs

Real space

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

In summary, we have presented DCA-QMC simulations with center-of-mass momentum

As noted, it is the

Figure 21 shows a plot of the leading eigenvalues

The fully irreducible vertex is essentially independent of $\epsilon$

Consistent with the Mermin-Wagner theorem, the finite

In summary, we have presented DCA-QMC simulations with center-of-mass momentum...
Spin-Fluctuation Pairing Interaction

\[ \Gamma^{pp}(\mathbf{k}, \omega_n, \mathbf{k}', \omega_{n'}) \approx \frac{3}{2} \bar{U}^2 \chi_s(\mathbf{k} - \mathbf{k}', \omega_n - \omega_{n'}) \]
Origin of Dome-Shaped $T_c$ vs. Doping

Separable approximation

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

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

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

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

\[ \mathcal{H} = \sum_{ij, \sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + V \sum_{\langle ij \rangle, \sigma\sigma'} n_{i\sigma} n_{j\sigma'} \]
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 $U \rightarrow$ additional nearest neighbor $V$ Coulomb repulsion

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

- $V$ is repulsive for nearest neighbor $d$-wave pairs
- Role of retardation?
DCA (QMC): $T_c$ versus $V$

$U = 7t$, $\langle n \rangle = 0.9$; 2 x 2 cluster

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

$\langle n \rangle = 0.9$

$T_c$ versus $V$ plot

Jiang et al., PRB '18
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 $T_c \sim 0.05t$ 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.