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Dynamic Cluster Approximation
LANL Summer School Lecture

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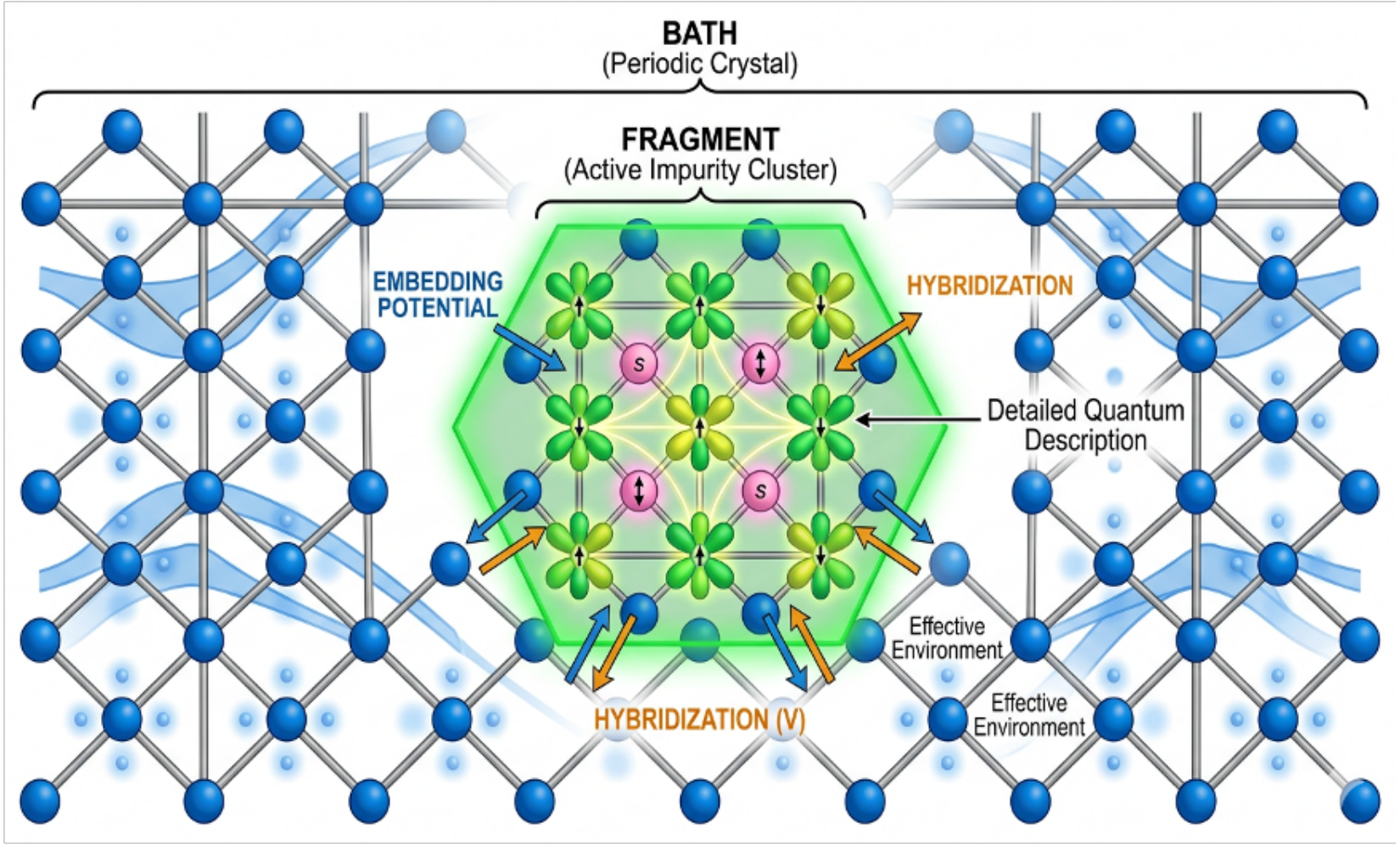
Quantum Embedding

The Takeaway Message



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Brief History

1989 – Dynamical Mean Field Theory (DMFT)

- Metzner & Vollhardt, Müller-Hartmann

1998 - 2000 – Dynamical Cluster Approximation (DCA)

- Jarrell et al.

2001 – Cellular DMFT

- Kotliar *et al.*

2000 – Cluster perturbation theory

- Sénéchal *et al.*, Gros & Valenti '93

DCA + related References

Original DCA papers

- Hettler, Tahvildar-Zadeh, Jarrell, Pruschke, Krishnamurthy, Phys. Rev. B 58, R747 (1998)
- Hettler, M. Mukherjee, Jarrell, Krishnamurthy, Phys. Rev. B 61, 12739 (2000)

Review paper (DCA, CDMFT, CPT)

- TAM, Jarrell, Pruschke, Hettler, Rev. Mod. Phys. 77, 1027 (2005)

Continuous time QMC cluster/impurity solvers

- Gull, Millis, Liechtenstein, Rubtsov, Troyer, Werner, Rev. Mod. Phys. 83, 349 (2011)

Corrections to Weiss Mean Field Theory

A Pedagogical Example

One dimensional Ising model

$$H = -J\sum_i \sigma_i\sigma_{i+1} - h\sum_i \sigma_i$$

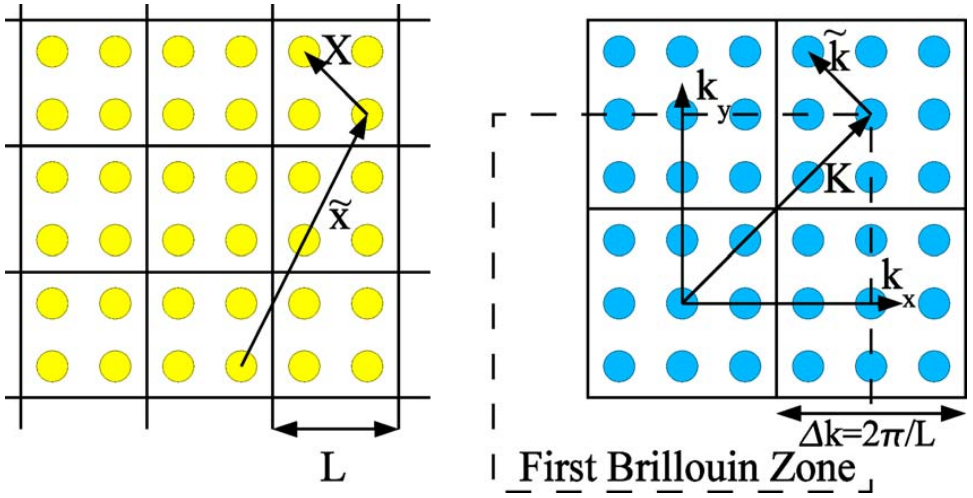
Intra- and inter-cluster

$$\mathbf{J}(\tilde{x}_i - \tilde{x}_j) = \mathbf{J}_c\delta_{\tilde{x}_i,\tilde{x}_j} + \delta\mathbf{J}(\tilde{x}_i - \tilde{x}_j)$$

Locator expansion for $\chi_{ij} = \beta(\langle\sigma_i\sigma_j\rangle - \langle\sigma_i\rangle\langle\sigma_j\rangle)$

$$\boldsymbol{\chi}(\tilde{x}_i - \tilde{x}_j) = \boldsymbol{\chi}^o\delta_{\tilde{x}_i,\tilde{x}_j} + \boldsymbol{\chi}^o\sum_l \delta\mathbf{J}(\tilde{x}_i - \tilde{x}_l)\boldsymbol{\chi}(\tilde{x}_l - \tilde{x}_j)$$

$$\boldsymbol{\chi}^o = \boldsymbol{\chi}(\delta\mathbf{J} = 0)$$



Superlattice Fourier-transform

$$\boldsymbol{\chi}(\tilde{q}) = \boldsymbol{\chi}^o + \boldsymbol{\chi}^o\delta\mathbf{J}(\tilde{q})\boldsymbol{\chi}(\tilde{q})$$

For single-site cluster this recovers standard Weiss mean-field theory

$$\chi(q=0) = \frac{1}{1/\chi^o - J(q=0)} = \frac{1}{T - T_c}$$

$$\chi^o = 1/T$$

$$\delta J(\tilde{q}=0) = J(q=0) = J$$

Corrections to Weiss Mean Field Theory

A Pedagogical Example

Translational symmetry violated since $\delta\mathbf{J}$ only couples surface sites; consider instead:

$$\chi(Q,\tilde{q}) = \chi^o(Q) + \chi^o(Q)\delta J(Q,\tilde{q})\chi(Q,\tilde{q}) \qquad \delta J(Q,\tilde{q}) = J(Q+\tilde{q}) - \bar{J}(Q),$$

$$= \frac{1}{1/\chi^o(Q) - \delta J(Q,\tilde{q})}, \qquad \bar{J}(Q) = \frac{N_c}{N}\sum_{\tilde{q}} J(Q+\tilde{q}).$$

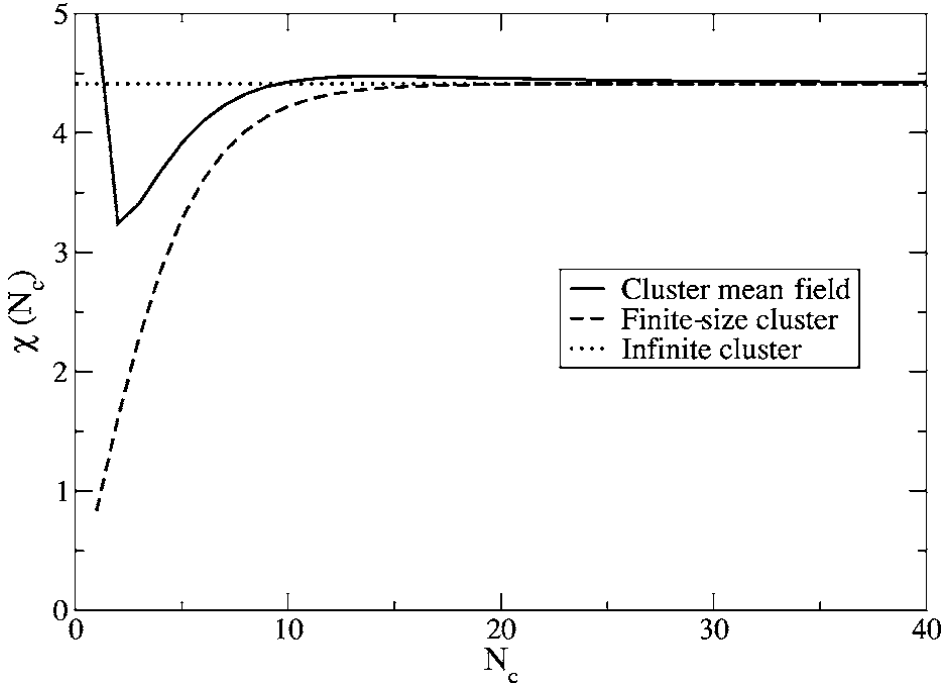
Solve analytically:

$$\bar{J}(Q=0) = J(N_c/\pi)\sin(\pi/N_c) \qquad \chi^o(Q=0) = \beta\exp(2K)\frac{1-[\tanh(K)]^{N_c}}{1+[\tanh(K)]^{N_c}}$$

$$K = \beta\bar{J}(Q=0) = \beta J(N_c/\pi)\sin(\pi/N_c)$$

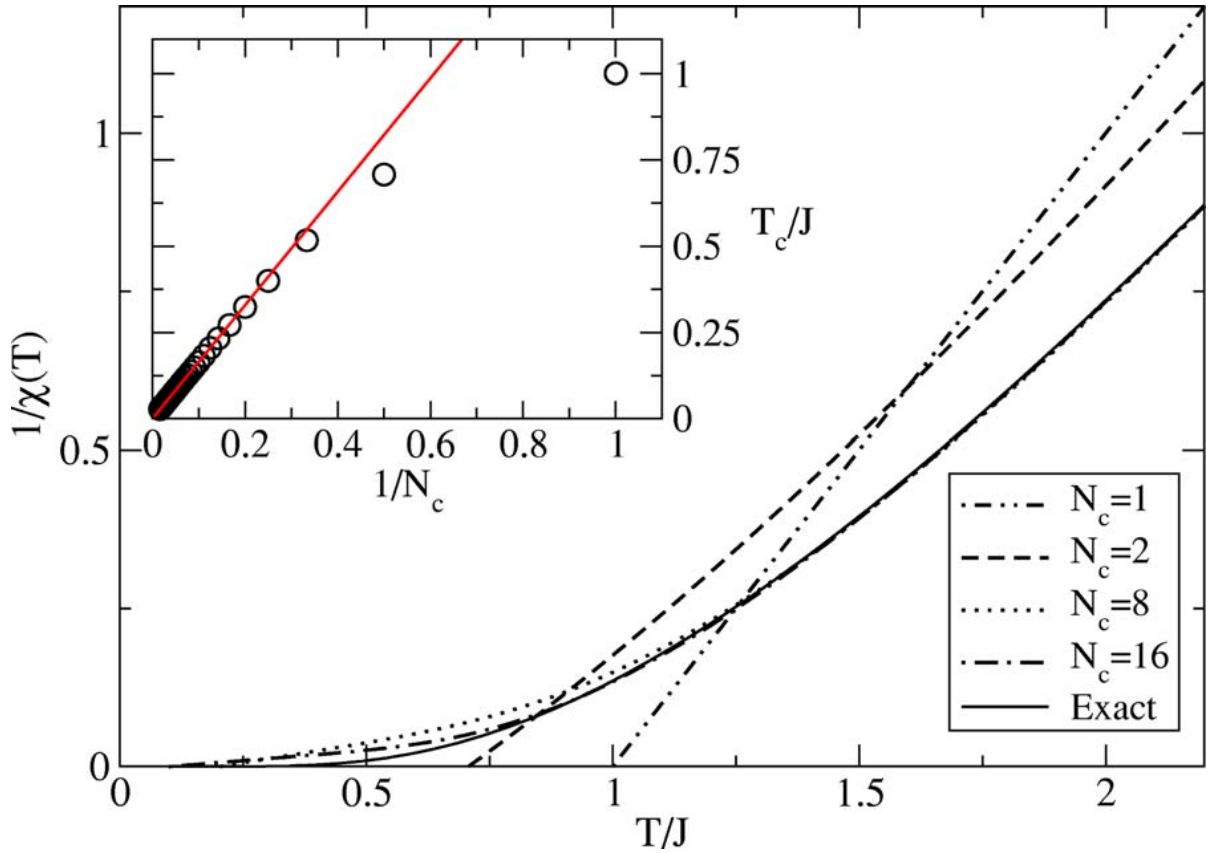
$$\chi(T) = \frac{1}{1/\chi^o(Q=0) - \delta J(Q=0,\tilde{q}=0)}$$

$$= \frac{1}{1/\chi^o(Q=0) - J[1-(N_c/\pi)\sin(\pi/N_c)]}$$



Corrections to Weiss Mean Field Theory

A Pedagogical Example



Mean-field behavior at low T: $\chi(T) \sim \frac{N_c}{T - T_c}$

Intermediate T:

$$\chi(T) \approx \beta e^{2\beta J}\left[1 - \frac{\beta J}{3}\left(\frac{\pi}{N_c}\right)^2\right] \quad \text{for } J \gg T \gg T_c$$

vs. exact result:

$$\chi(T) \approx \beta \exp(2\beta J)$$

Notes / Observations

Also true for dynamical cluster approximation

Cluster mean-field solution interpolates between single-site mean-field and infinite cluster exact result

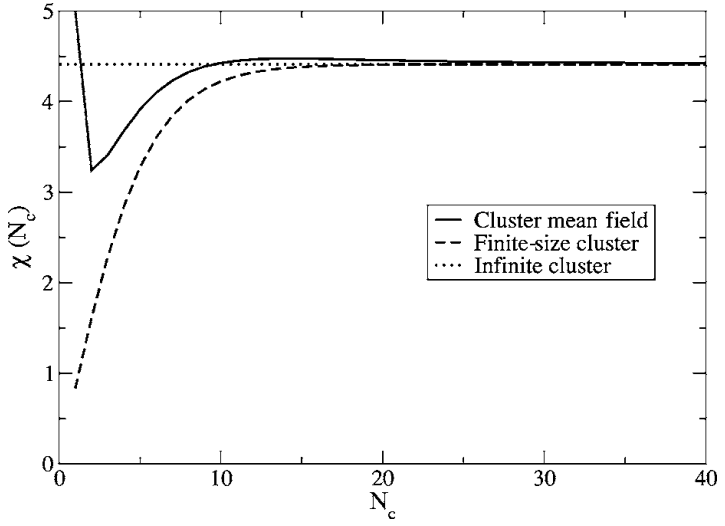
Cluster size convergence to exact result is faster than in finite size methods; for a given cluster size, cluster mean-field theories give better approximation

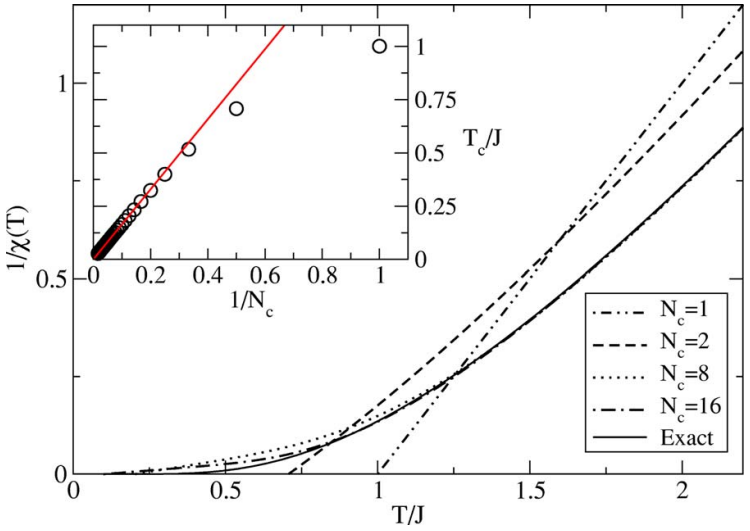
(Cluster) mean-field treatment of long wavelength fluctuations results in finite transition temperature, even if exact transition temperature is zero

With increasing cluster size, transition temperature is suppressed by inclusion of longer wavelength fluctuations

Intermediate temperature regime reflects temperature dependence of exact result (infinite size clusters)

Finite size scaling can be performed if sufficiently large clusters can be simulated





Dynamic Cluster Approximation

Preliminaries

2D Hubbard model

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

Thermodynamic Green's function

$$G_{ij,\sigma} = -\langle T_\tau c_{i\sigma}(\tau) c^{\dagger}_{j\sigma} \rangle \; ; \; G_{ij,\sigma}(i\omega_n) = \int_0^\beta d\tau \, e^{i\omega_n \tau} G_{ij,\sigma}(\tau) \, , \; \omega_n = (2n+1)\pi T$$

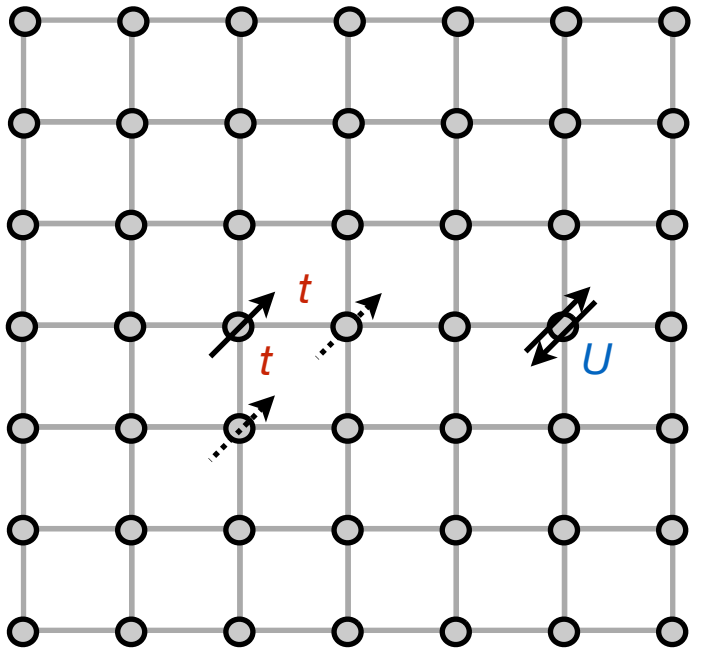
$$G_\sigma(\mathbf{k}, i\omega_n) \equiv \langle\langle c_{\mathbf{k},\sigma} ; c^{\dagger}_{\mathbf{k},\sigma} \rangle\rangle_{i\omega_n} = \frac{1}{N} \sum_{ij} e^{i\mathbf{k}(\mathbf{r}_i - \mathbf{r}_j)} G_{ij,\sigma}(i\omega_n)$$

Green's function of non-interacting system (U=0)

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

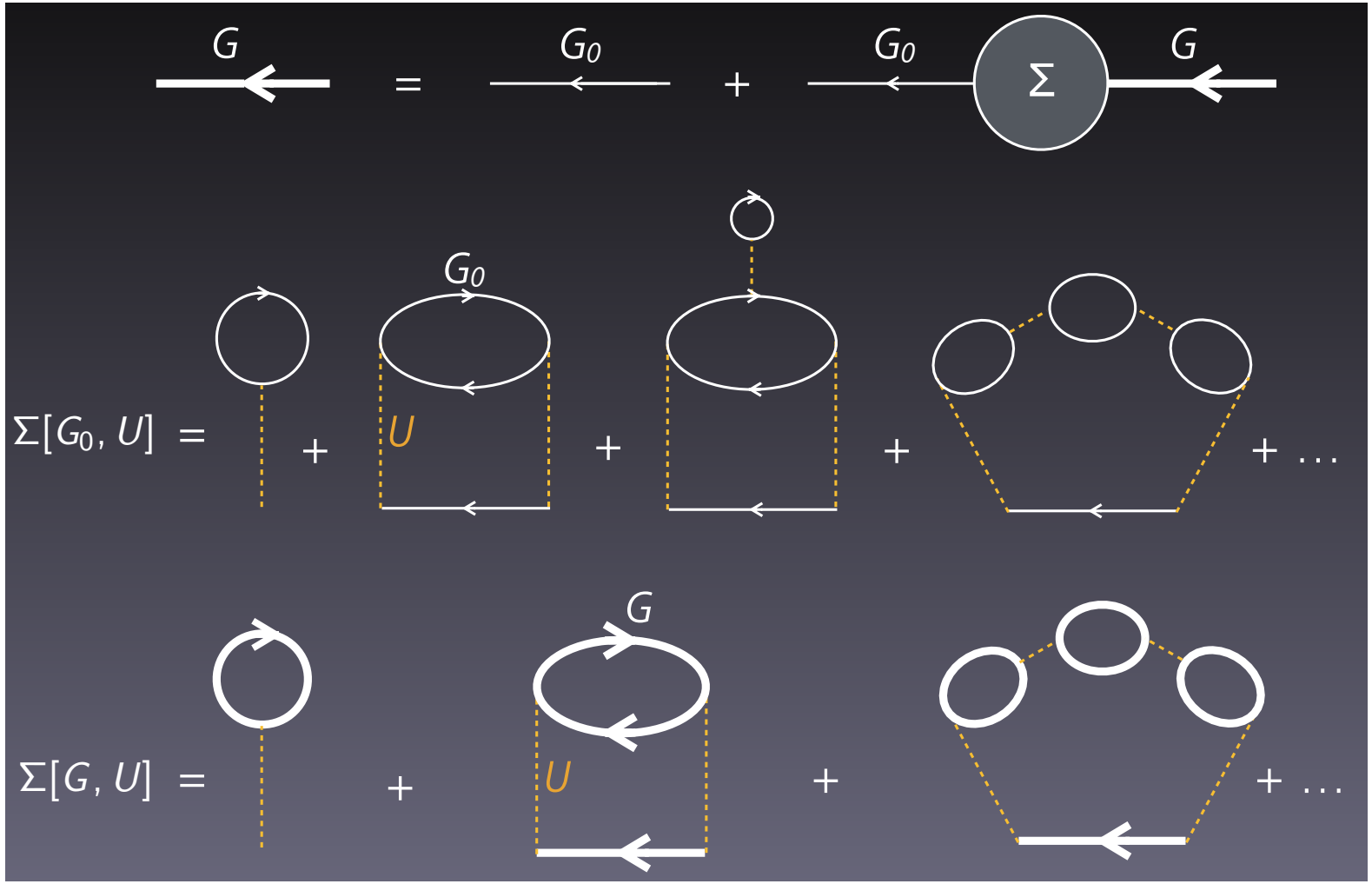
Dyson equation defines self-energy $\Sigma(\mathbf{k}, i\omega_n)$

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



Dyson equation for Green's function

$$\Sigma = \mathscr{F}[G]$$



Action / Lagrangian

More natural formalism for dynamics

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

- Action

$$S[\phi^*, \phi] = -\int_0^\beta d\tau \int_0^\beta d\tau' \sum_{\mathbf{k},\sigma} \phi^*_{\mathbf{k}\sigma}(\tau) G^{-1}_{0,\sigma}(\mathbf{k}, \tau - \tau') \phi_{\mathbf{k}\sigma}(\tau) + \int_0^\beta d\tau \sum_i U \phi^*_{i\uparrow}(\tau) \phi_{i\uparrow} \phi^*_{i\downarrow}(\tau) \phi_{i\downarrow}(\tau)$$

- Interacting Green's function

$$G_{c,\sigma}(\mathbf{k}, \tau - \tau') = \frac{1}{Z} \int \mathcal{D}[\phi^* \phi] \phi_{\mathbf{k}\sigma}(\tau) \phi^*_{\mathbf{k}\sigma}(\tau') e^{-S[\phi^*, \phi]}$$

Dynamic Cluster Approximation

Locator Approach

Intra- and inter-cluster hopping / self-energy:

$$\mathbf{t}(\tilde{\mathbf{x}}_i - \tilde{\mathbf{x}}_j) = \mathbf{t}_c \delta_{\tilde{\mathbf{x}}_i,\tilde{\mathbf{x}}_j} + \delta\mathbf{t}(\tilde{\mathbf{x}}_i - \tilde{\mathbf{x}}_j),$$

$$\boldsymbol{\Sigma}(\tilde{\mathbf{x}}_i - \tilde{\mathbf{x}}_j, z) = \boldsymbol{\Sigma}_c(z)\,\delta_{\tilde{\mathbf{x}}_i,\tilde{\mathbf{x}}_j} + \delta\boldsymbol{\Sigma}(\tilde{\mathbf{x}}_i - \tilde{\mathbf{x}}_j, z)$$

Locator expansion for Green's function

$$\mathbf{G}(\tilde{\mathbf{x}}_i - \tilde{\mathbf{x}}_j, z) = \mathbf{g}(z)\,\delta_{\tilde{\mathbf{x}}_i\tilde{\mathbf{x}}_j} + \mathbf{g}(z)\sum_l [\,\delta\mathbf{t}(\tilde{\mathbf{x}}_i - \tilde{\mathbf{x}}_l) + \delta\boldsymbol{\Sigma}(\tilde{\mathbf{x}}_i - \tilde{\mathbf{x}}_l, z)]\mathbf{G}(\tilde{\mathbf{x}}_l - \tilde{\mathbf{x}}_j, z),$$

$$\mathbf{g}(z) = [(z+\mu)\mathbb{1} - \mathbf{t}_c - \boldsymbol{\Sigma}_c(z)]^{-1}$$

Superlattice Fourier-transform

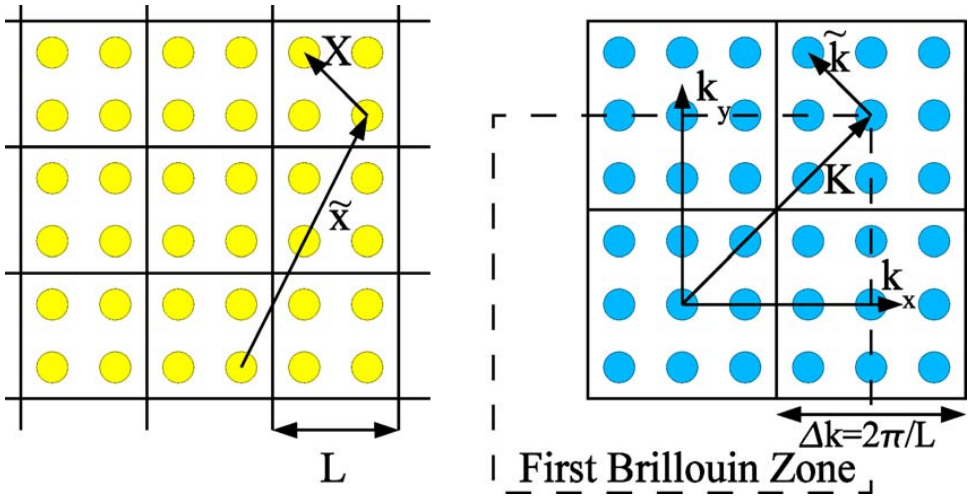
$$\mathbf{G}(\tilde{\mathbf{k}}, z) = \mathbf{g}(z) + \mathbf{g}(z)[\,\delta\mathbf{t}(\tilde{\mathbf{k}}) + \delta\boldsymbol{\Sigma}(\tilde{\mathbf{k}}, z)]\mathbf{G}(\tilde{\mathbf{k}}, z)$$

Central Approximation: $\delta\Sigma = 0$

$$\mathbf{G}(\tilde{\mathbf{k}}, z) = \mathbf{g}(z) + \mathbf{g}(z)\,\delta\mathbf{t}(\tilde{\mathbf{k}})\mathbf{G}(\tilde{\mathbf{k}}, z) = [\mathbf{g}^{-1}(z) - \delta\mathbf{t}(\tilde{\mathbf{k}})]^{-1}$$

$$\boldsymbol{\Sigma}_c(z) = \mathcal{F}[\bar{\mathbf{G}}(z)]$$

$$\bar{\mathbf{G}}(z) = \frac{N_c}{N}\sum_{\tilde{\mathbf{k}}} \mathbf{G}(\tilde{\mathbf{k}}, z)$$



Dynamic Cluster Approximation

How to restore translational invariance

$$[\mathbf{t}(\tilde{\mathbf{k}})]_{\mathbf{X}_i\mathbf{X}_j} = \frac{1}{N_c}\sum_{\mathbf{K}} e^{i(\mathbf{K}+\tilde{\mathbf{k}})\cdot(\mathbf{X}_i-\mathbf{X}_j)}\epsilon_{\mathbf{K}+\tilde{\mathbf{k}}}$$

Phase factors $e^{i\tilde{\mathbf{k}}\cdot(\mathbf{X}_i-\mathbf{X}_j)}$ break translational symmetry in cluster

Use $[\mathbf{t}_{\mathrm{DCA}}(\tilde{\mathbf{k}})]_{\mathbf{X}_i\mathbf{X}_j} = [\mathbf{t}(\tilde{\mathbf{k}})]_{\mathbf{X}_i\mathbf{X}_j} e^{-i\tilde{\mathbf{k}}\cdot(\mathbf{X}_i-\mathbf{X}_j)}$

$$= \frac{1}{N_c}\sum_{\mathbf{K}} e^{i\mathbf{K}\cdot(\mathbf{X}_i-\mathbf{X}_j)}\epsilon_{\mathbf{K}+\tilde{\mathbf{k}}}$$

instead, to restore translational invariance

$$[\mathbf{t}_{c,\mathrm{DCA}}]_{\mathbf{X}_i\mathbf{X}_j} = \frac{1}{N_c}\sum_{\mathbf{K}} e^{i\mathbf{K}\cdot(\mathbf{X}_i-\mathbf{X}_j)}\bar{\epsilon}_{\mathbf{K}} \qquad \bar{\epsilon}_{\mathbf{K}} = \frac{N_c}{N}\sum_{\tilde{\mathbf{k}}} \epsilon_{\mathbf{K}+\tilde{\mathbf{k}}}$$

$$[\delta\mathbf{t}_{\mathrm{DCA}}(\tilde{\mathbf{k}})]_{\mathbf{X}_i\mathbf{X}_j} = \frac{1}{N_c}\sum_{\mathbf{K}} e^{i\mathbf{K}\cdot(\mathbf{X}_i-\mathbf{X}_j)}\delta t(\mathbf{K}+\tilde{\mathbf{k}}) \qquad \delta t(\mathbf{K}+\tilde{\mathbf{k}}) = \epsilon_{\mathbf{K}+\tilde{\mathbf{k}}} - \bar{\epsilon}_{\mathbf{K}}$$

$$G(\mathbf{K}+\tilde{\mathbf{k}},z) = g(\mathbf{K},z) + g(\mathbf{K},z)\,\delta t(\mathbf{K}+\tilde{\mathbf{k}})G(\mathbf{K}+\tilde{\mathbf{k}},z)$$

$$= \frac{1}{g^{-1}(\mathbf{K},z) - \delta t(\mathbf{K}+\tilde{\mathbf{k}})}, \qquad g(\mathbf{K},z) = [z - \bar{\epsilon}_{\mathbf{K}} + \mu - \Sigma_c(\mathbf{K},z)]^{-1}$$

Coarse-grained Green's function

$$\bar{G}(\mathbf{K},z) = \frac{N_c}{N}\sum_{\tilde{\mathbf{k}}} G(\mathbf{K}+\tilde{\mathbf{k}},z) = \frac{1}{g^{-1}(\mathbf{K},z) - \Gamma(\mathbf{K},z)}$$

$$\Gamma(\mathbf{K},z) = \frac{\frac{N_c}{N}\sum_{\tilde{\mathbf{k}}} \delta t^2(\mathbf{K}+\tilde{\mathbf{k}})G(\mathbf{K}+\tilde{\mathbf{k}},z)}{1 + \frac{N_c}{N}\sum_{\tilde{\mathbf{k}}} \delta t(\mathbf{K}+\tilde{\mathbf{k}})G(\mathbf{K}+\tilde{\mathbf{k}},z)}$$

Homework problem

$$\bar{G}(\mathbf{K},z) = [G_0(\mathbf{K},z) - \Sigma_c(\mathbf{K},z)]^{-1}$$

$$\Sigma_c(\mathbf{K},z) = \mathscr{F}[\bar{G}(\mathbf{K},z)]$$

Dynamic Cluster Approximation

Nature of effective cluster problem

Consider 1D model

$$\mathbf{t}_{c,\mathrm{DCA}} = N_c/N \Sigma_{\tilde{k}} \mathbf{t}_{\mathrm{DCA}}(\tilde{k})$$

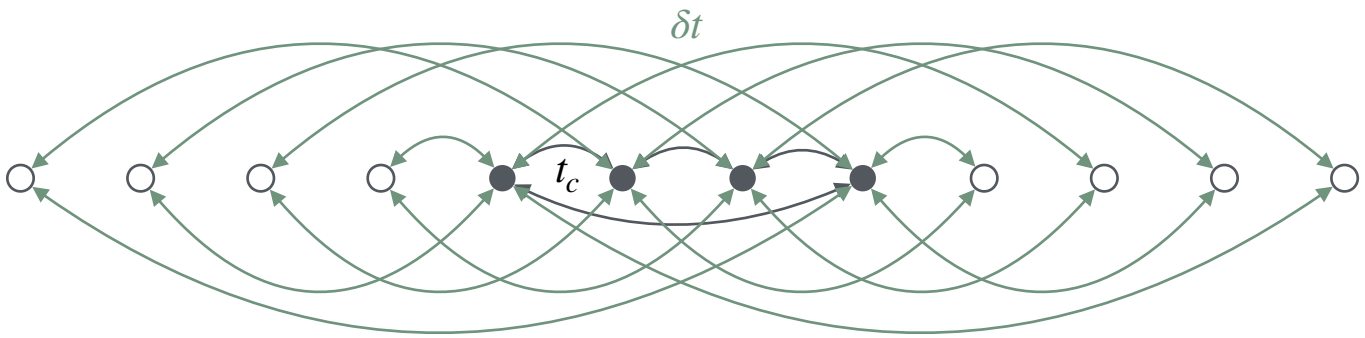
$$[\mathbf{t}_{c,\mathrm{DCA}}]_{X_i,X_j} = -t\frac{L_c}{\pi}\sin\frac{\pi}{L_c}$$

$$[\delta\mathbf{t}_{\mathrm{DCA}}(\tilde{x})]_{X_i X_j} = -t\left(\frac{\sin[(\tilde{x}\mp 1)\pi/L_c]}{(\tilde{x}\mp 1)\pi/L_c} - \frac{\sin(\pi/L_c)}{\pi/L_c}\delta_{\tilde{x},0}\right)$$

$\delta\mathbf{t}_{\mathrm{DCA}} \sim 1/L_c$ for large $\boldsymbol{L_c}$

$$\Gamma \sim \mathcal{O}(\frac{1}{L_c^2})$$

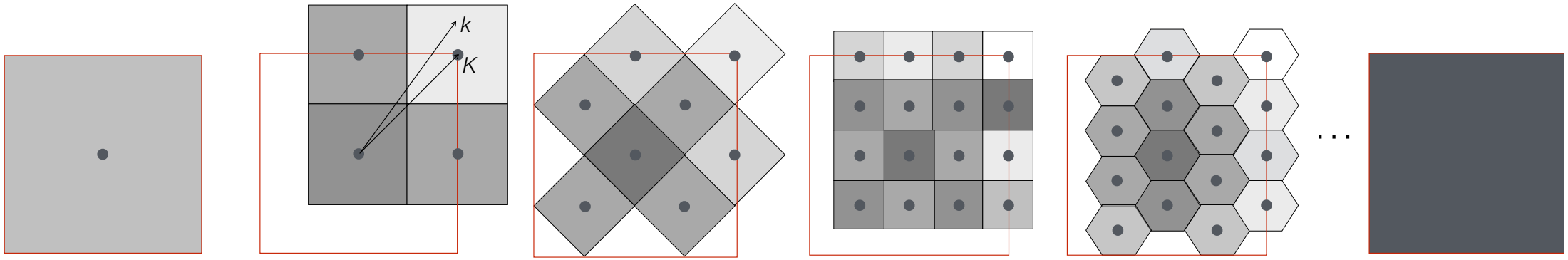
$$\Sigma \approx \Sigma_{DCA} + \mathcal{O}(\frac{1}{L_c^2})$$



Cluster has reduced intra-cluster hopping t_c, but every site in the cluster is coupled to neighboring site in the effective medium

Dynamic Cluster Approximation

Coarse-graining



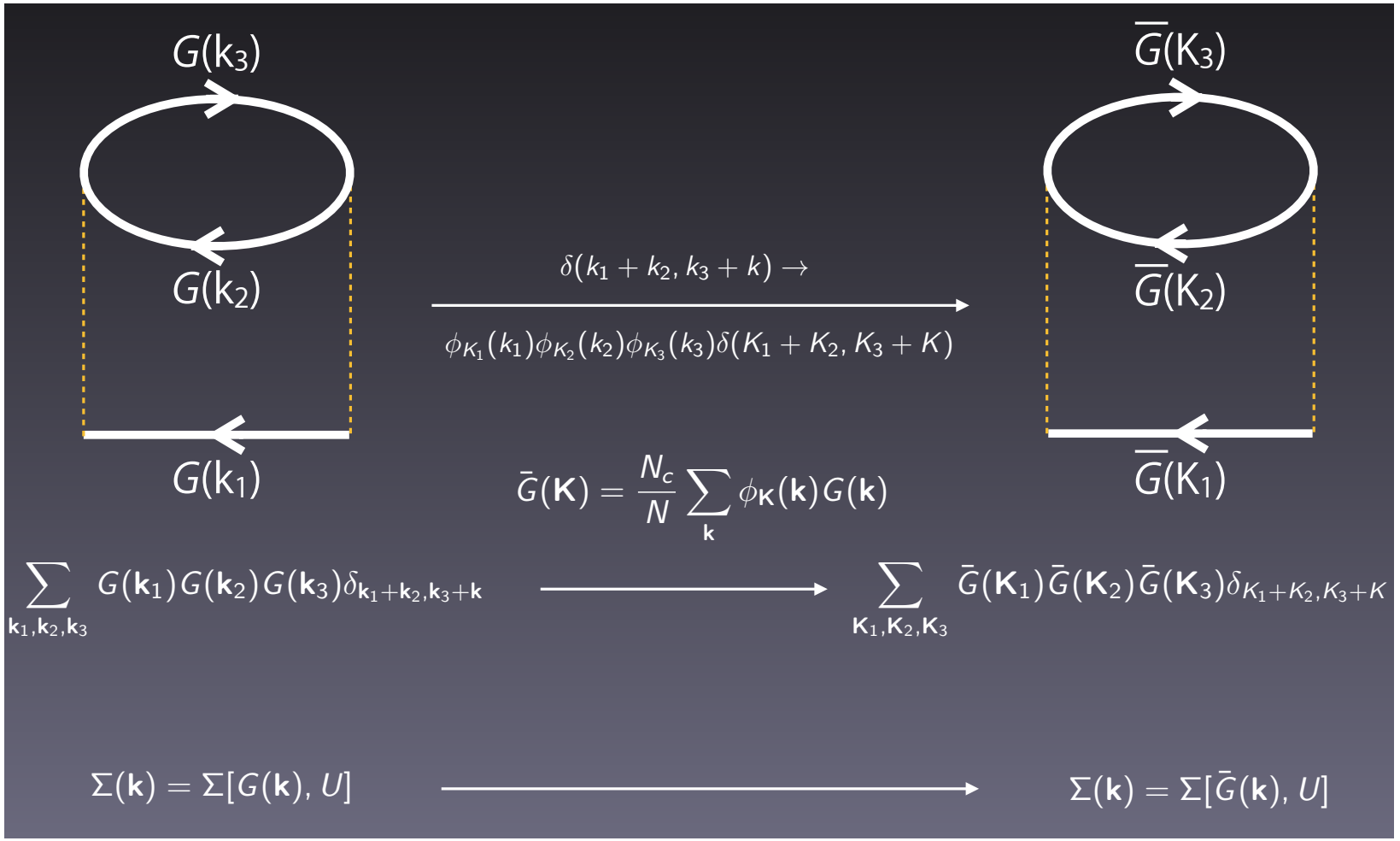
General idea: Represent bulk system by reduced number of cluster degrees of freedom, and use coarse graining to retain information about remaining degrees of freedom

$$\Sigma(k,z) \approx \Sigma_c(K,z) + \delta\Sigma(K,k',z)$$

$$\Sigma_c(K,z) = \mathcal{F}[\bar{G}(K,z)]$$

$$\bar{G}(K,z) = \frac{N_c}{N}\sum_{k'} G(K+k',z)$$

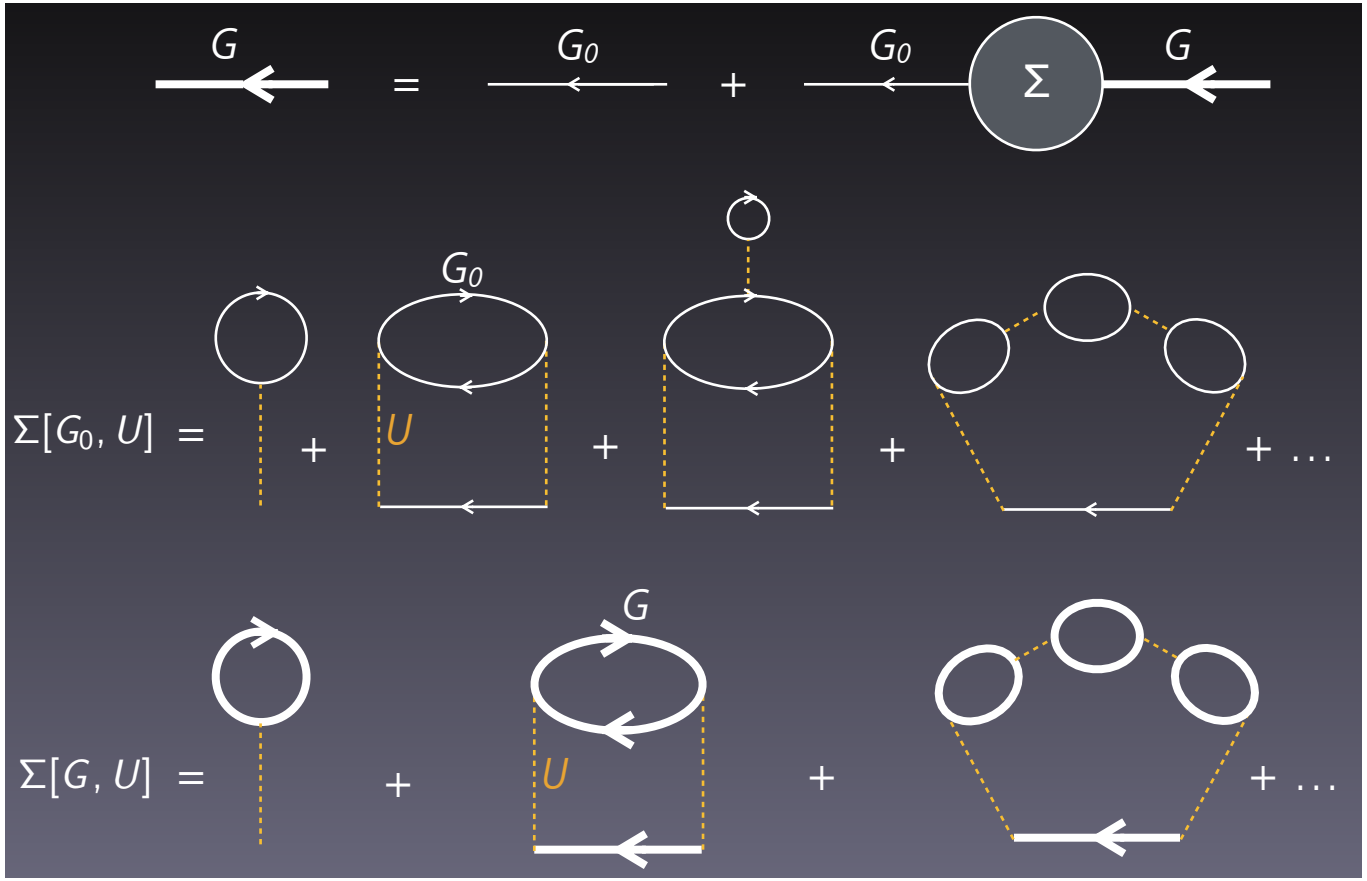
Coarse graining



Momentum conservation for cluster momenta K only

“Cluster Exclusion”

Bare diagram expansion vs. skeleton expansion



Requires additional “cluster exclusion step”:

$$\mathcal{G}_0(K,z) = [\bar{G}(K,z) + \Sigma_c(K,z)]^{-1}$$

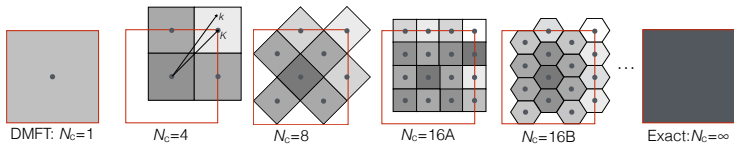
Effective medium Green’s function = bare cluster Green’s function, i.e., with correlations removed

Dynamic Cluster Approximation

Iterative procedure for self-consistency

(1) Coarse-graining

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



(2) Cluster exclusion

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

(3) Cluster problem solution

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

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

(4) New self-energy

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

Quantum Monte Carlo (QMC) cluster solver

State-of-the-art: Continuous time QMC

Excellent review of continuous-time QMC solvers:

- *E. Gull et al., Continuous-time Monte Carlo methods for quantum impurity models, Rev. Mod. Phys. 83, 349-404 (2011)*

Interaction (U) expansion, hybridization (Γ) expansion, and auxiliary field algorithms

Continuous time auxiliary field (CT-AUX) QMC employs auxiliary field decoupling of interaction term, then performs Monte Carlo sampling of expansion in interaction U

CT-AUX QMC

- Auxiliary field decomposition

$$1 - \frac{\beta U}{K} \sum_i \left[n_{i\uparrow} n_{i\downarrow} - \frac{1}{2}(n_{i\uparrow} + n_{i\downarrow}) \right] = \frac{1}{2N_c} \sum_{i, s_i = \pm 1} e^{\gamma s_i (n_{i\uparrow} - n_{i\downarrow})} \; ; \quad \cosh(\gamma) = 1 + \frac{U\beta N_c}{2K}$$

- Partition function

$$Z = \sum_{k=0}^{\infty} \sum_{s_1 \ldots s_k = \pm 1} \int_0^\beta d\tau_1 \ldots \int_{\tau_{k-1}}^\beta d\tau_k \left(\frac{K}{2\beta N_c} \right)^k Z_k(\{x, \tau, s\}_k)$$

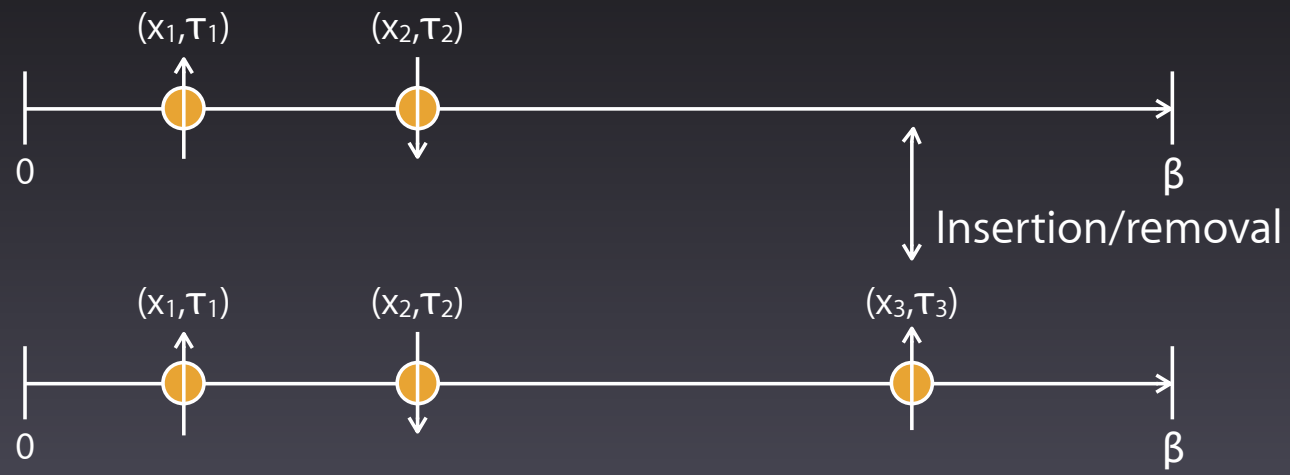
- Sum over expansion orders

$$Z_k(\{x, \tau, s\}_k) = Z_0 \prod_\sigma \det N_\sigma^{-1}(\{x, \tau, s\}_k) \; ; \; [N_\sigma^{-1}]_{ij} = e^{\gamma(-1)^\sigma s_i} \delta_{ij} - \mathcal{G}_{0,\sigma}(x_i, \tau_i; x_j, \tau_j)(e^{\gamma(-1)^\sigma s_i} - \delta_{ij})$$

- Monte Carlo sampling space

QMC Updates

Insertion and removal updates



Probability for updating configuration x to x'

$$R_{x\to x'} = \min(1, R)\,;\; R = \frac{K}{k+1}\prod_{\sigma}\frac{\det \mathbf{N}_{\sigma}^{-1}(\{x', \tau', s'\})}{\det \mathbf{N}_{\sigma}^{-1}(\{x, \tau, s\})}$$

Measurement of Green's function

$$G_{pq}(\tau, \tau') = \frac{1}{Z}\sum_{k=0}^{\infty}\sum_{s_1 \ldots s_k = \pm 1}\int_0^{\beta} d\tau_1 \ldots \int_{\tau_{k-1}}^{\beta} d\tau_k \left(\frac{K}{2\beta N_c}\right)^k Z_k(\{x, \tau, s\}_k)\tilde{G}_{pq}^{\{x,\tau,s\}_k}(\tau, \tau')$$

$$\tilde{G}_{pq}(\tau, \tau') = [\mathbf{N}\mathcal{G}_0]_{pq}$$

Fermion Sign Problem

- Weights of configurations can be negative

$$A = \frac{1}{Z}\int dx\, A(x)p(x) = \frac{1}{Z}\frac{\int dx\, A(x)|p(x)|sgn(x)}{\int dx\, sgn(x)|p(x)|} = \frac{\langle A\rangle_{|p|}}{\langle sgn\rangle_{|p|}}$$

- Average sign

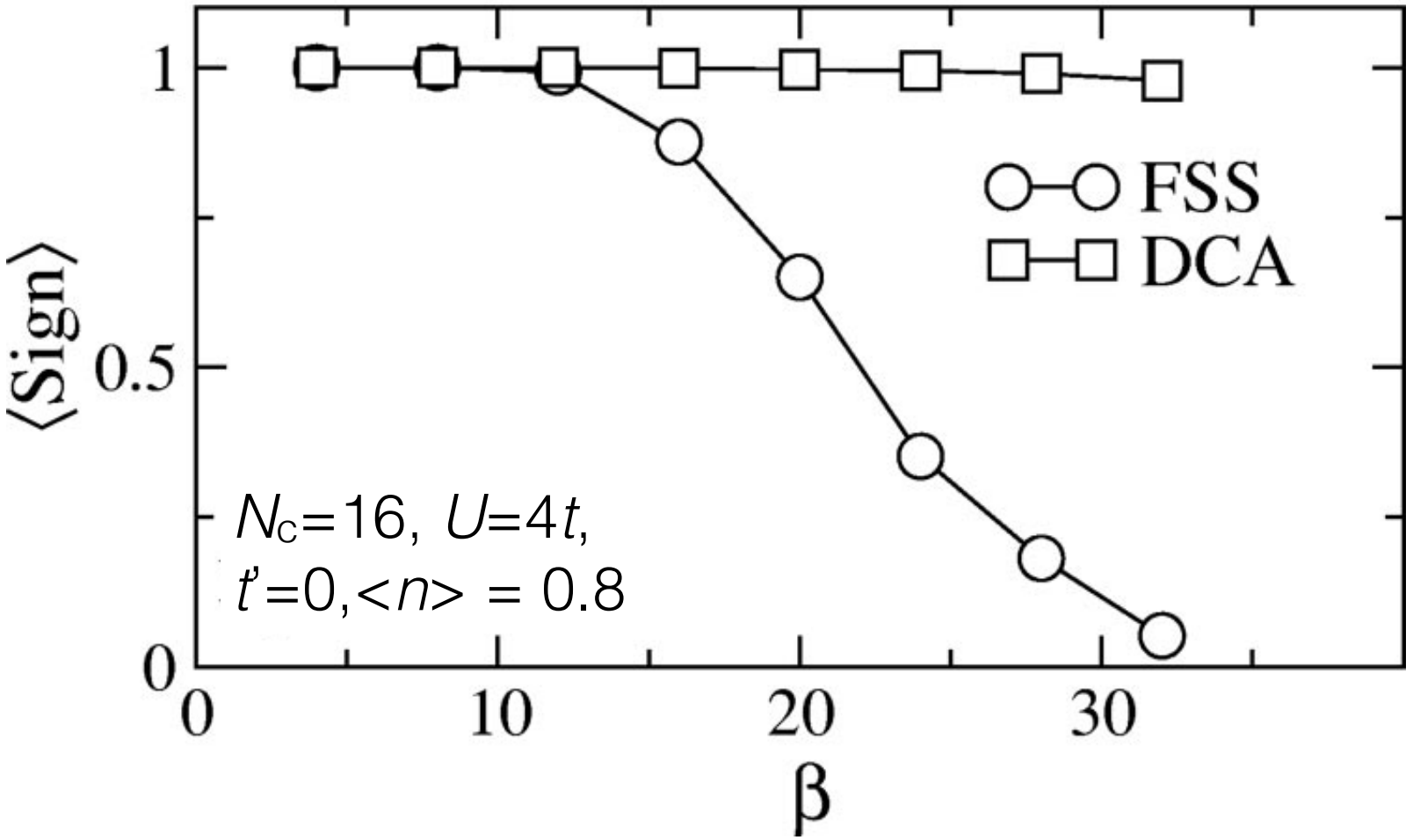
$$\langle sgn\rangle = \frac{\int dx\, sgn(x)|p(x)|}{\int dx\, |p(x)|} = \frac{Z}{Z_{|p|}}$$

- Ratio of Z and $Z_{|p|}$ of "bosonic" system with positive weights

$$\frac{Z}{Z_{|p|}} = \exp(-\beta\Delta F)$$

- Average sign decreases exponentially with system size, inverse temperature and U and leads to exponential statistical errors.

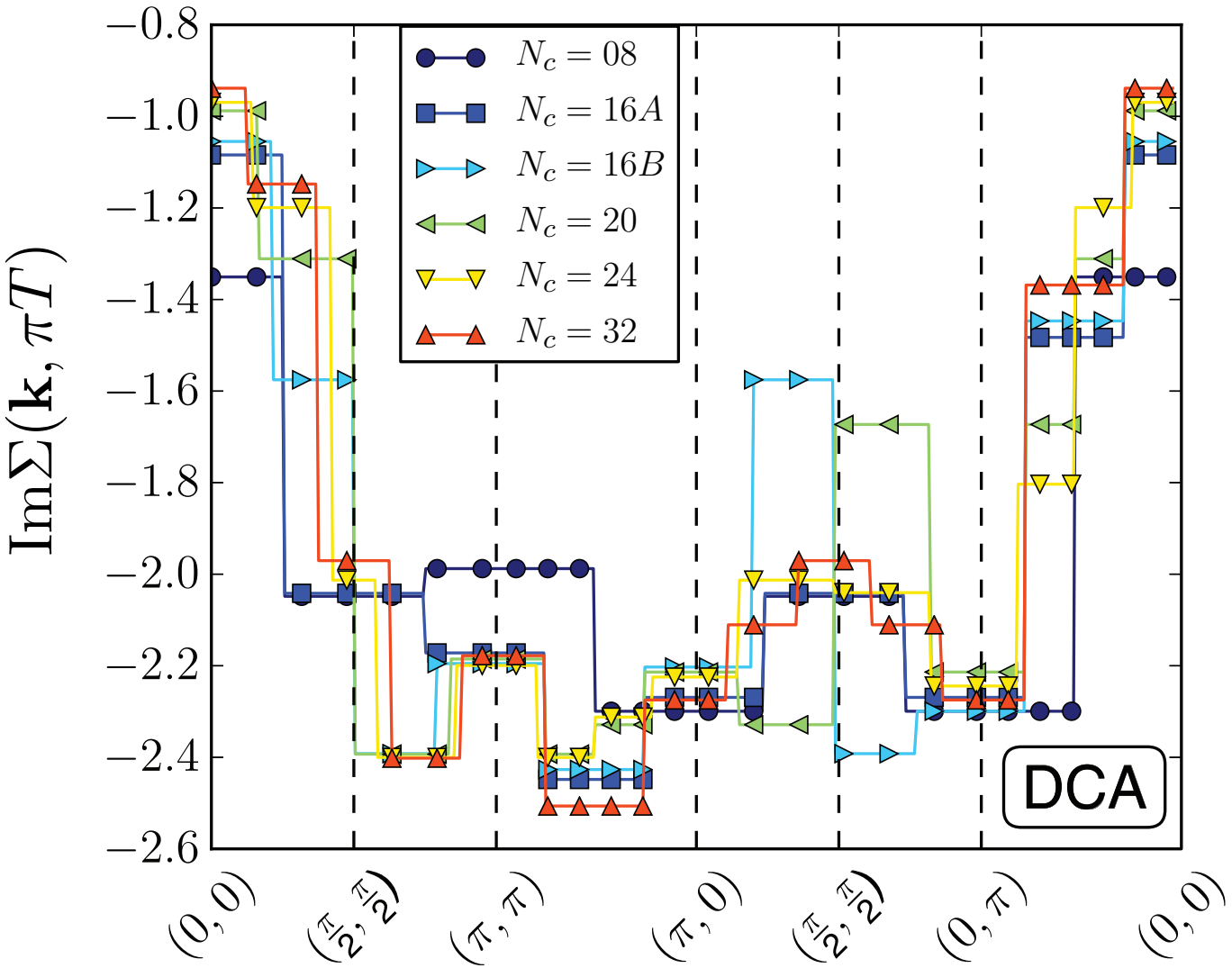
Fermion Sign Problem



DCA/QMC has much weaker sign problem than finite size QMC calculations

DCA self-energy

Piecewise constant approximation



Symmetry broken phases

Two approaches

1. Apply symmetry breaking field and calculate "anomalous" Green's function, e.g., for superconducting phases:

$$F_{ij}(\tau) = -\langle T_\tau c_{i\uparrow}(\tau) c_{j\downarrow}(0)\rangle; \quad P_s = \left.\frac{\partial \Delta_s}{\partial \Psi}\right|_{\Psi=0}; \quad \Delta_s = \frac{T}{N}\sum_{k,i\omega_n} F(k, i\omega_n)$$

2. Calculate susceptibility from two-particle correlation function

$$P_s = \int_0^\beta d\tau \langle \Delta_s(\tau)\Delta_s^\dagger(0)\rangle$$

DCA is "thermodynamically consistent" → two approaches give identical results

Superconductivity

The Basics

Phenomenology

- First discovered in Hg by Kamerlingh Onnes (1911)
- Perfect conductivity (zero resistance)
- Perfect diamagnetism (Meissner-Ochsenfeld effect, 1933)
  $\longrightarrow$ 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

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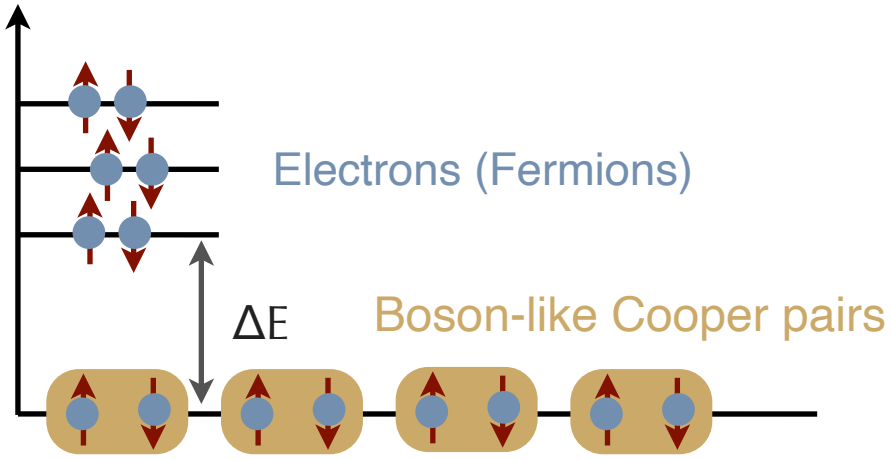
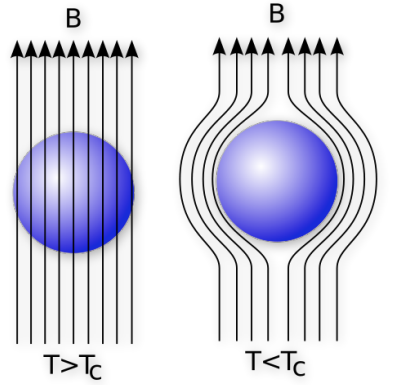
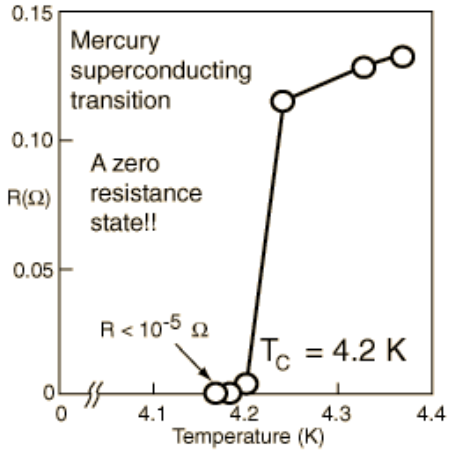


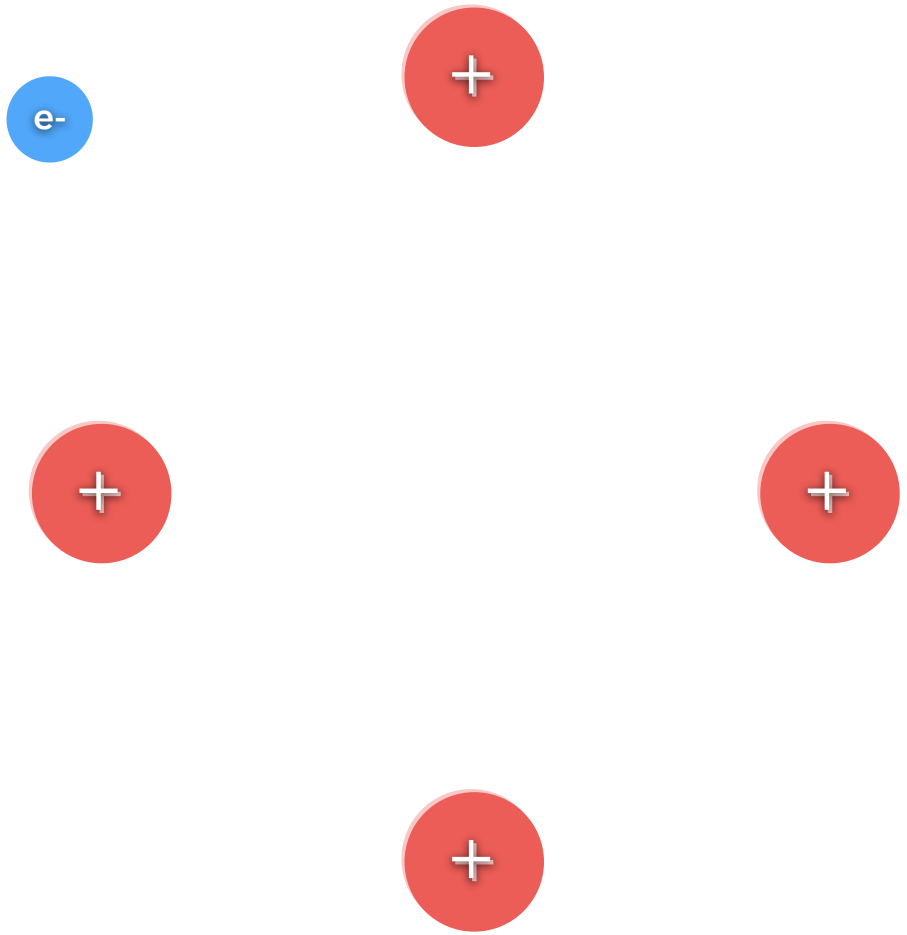




Bardeen Cooper Schrieffer

Pair Formation in Conventional Superconductors

The electron-phonon mechanism



Pair Formation in Conventional Superconductors

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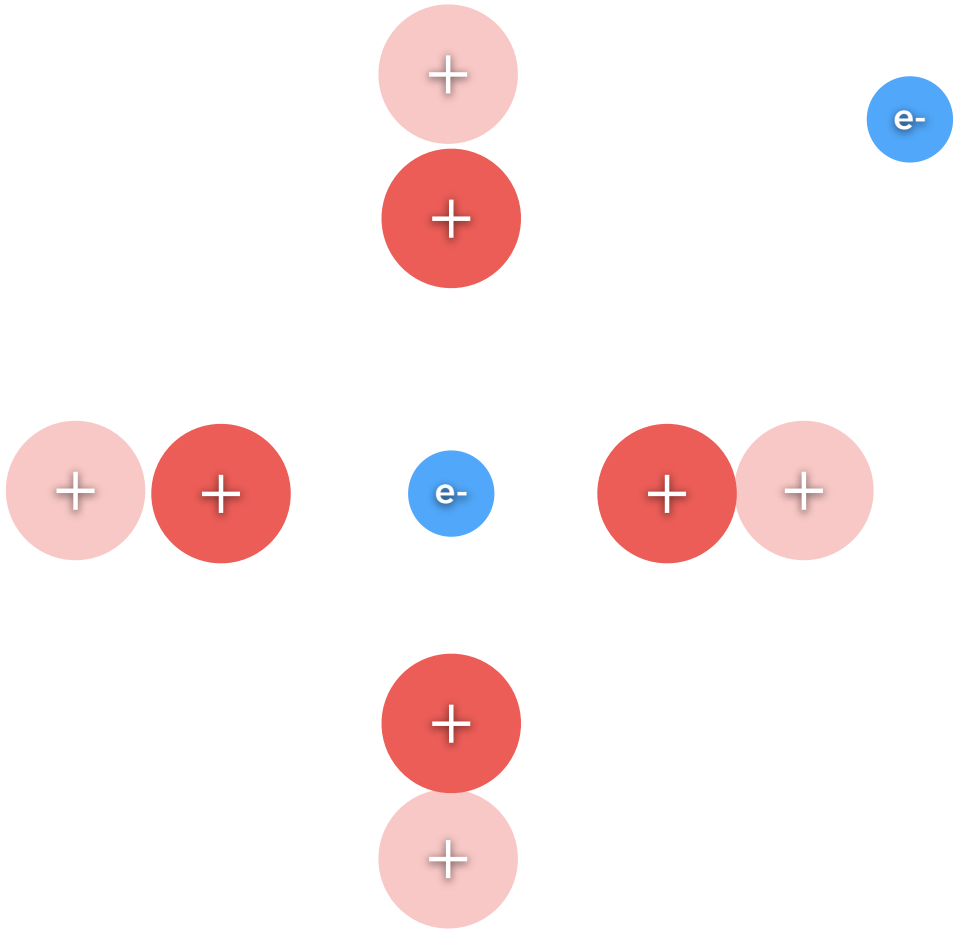
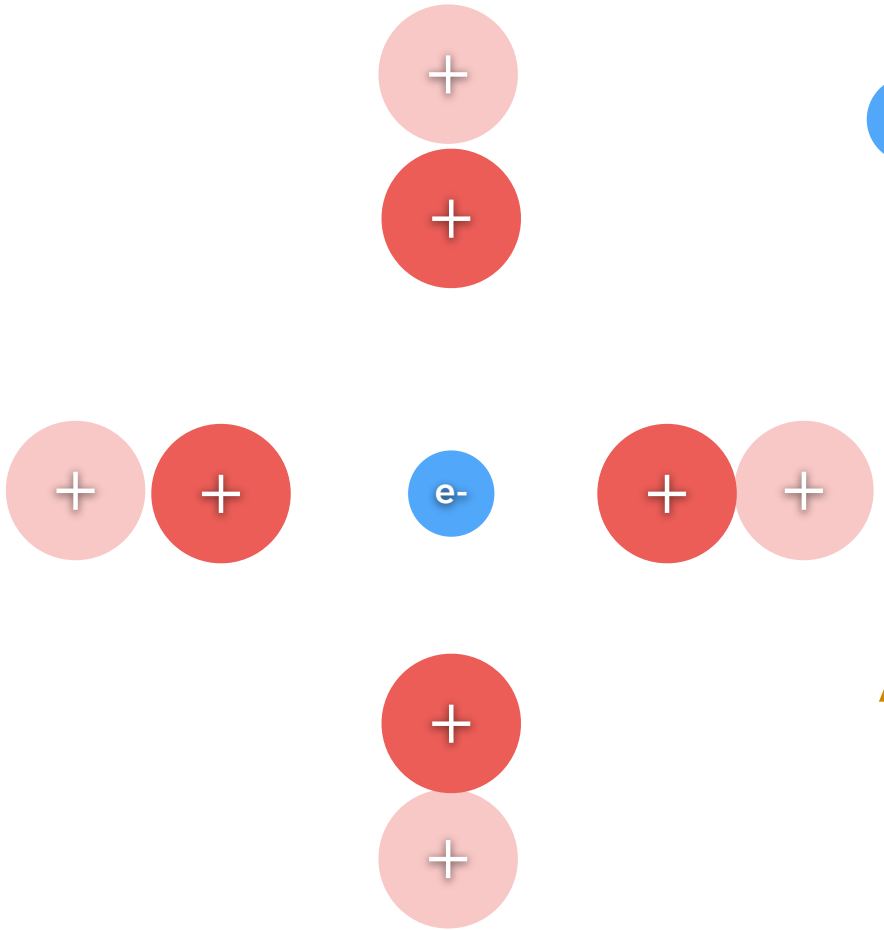


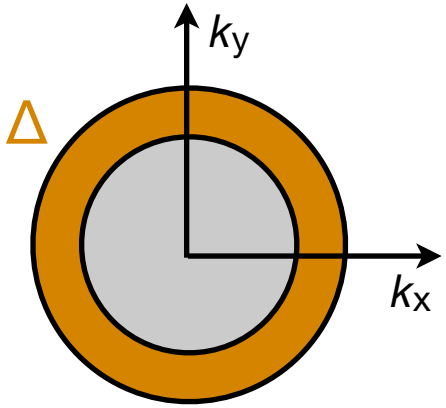
Pair Formation in Conventional Superconductors

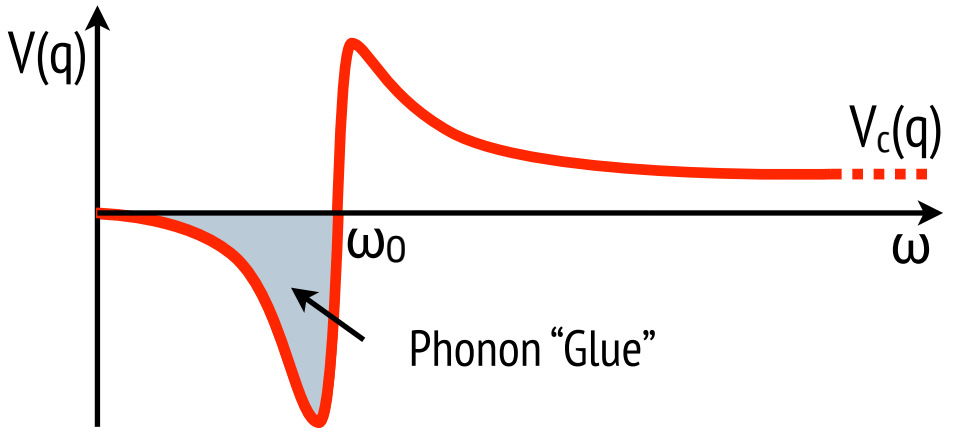
The electron-phonon mechanism



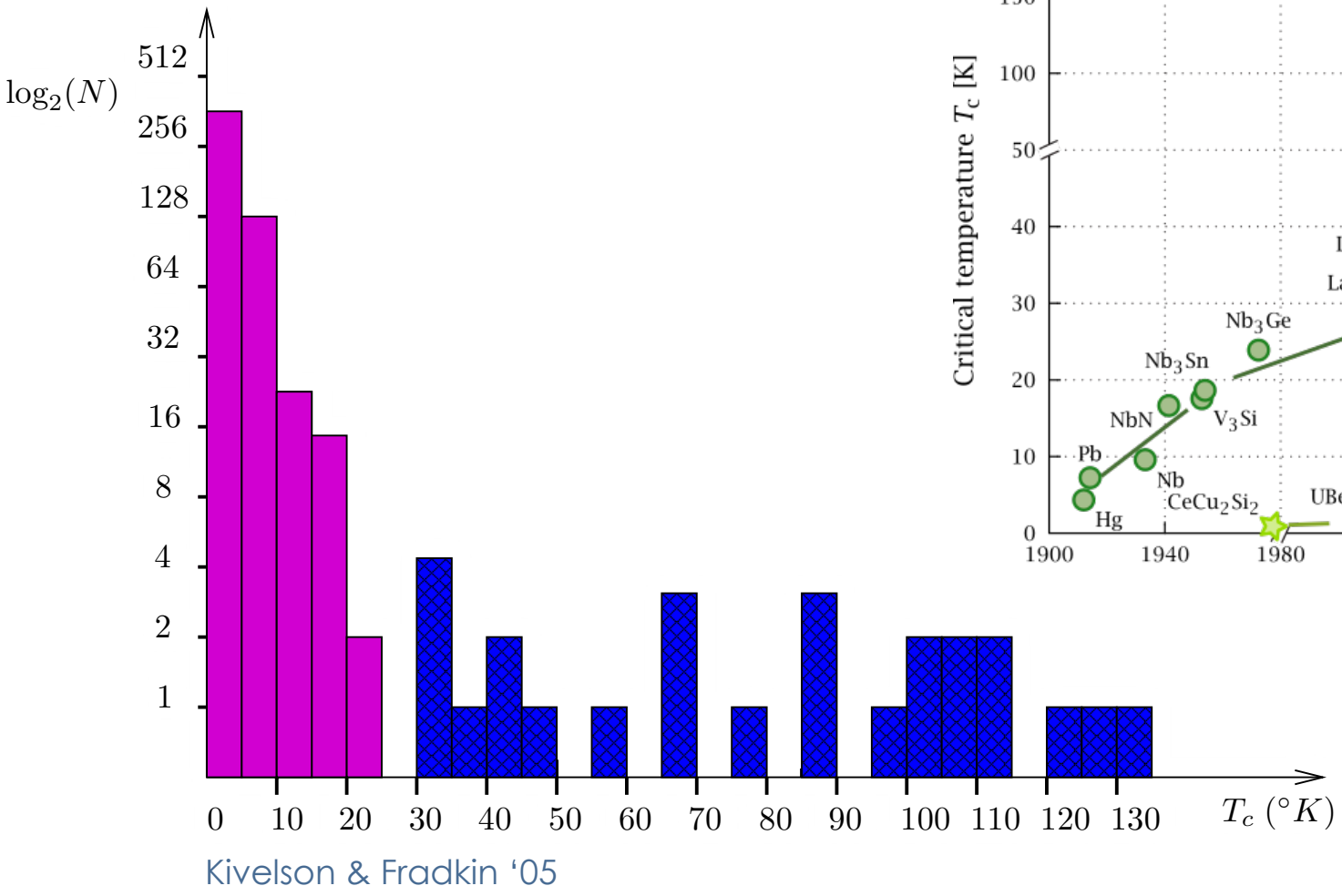
Phonon mechanism

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



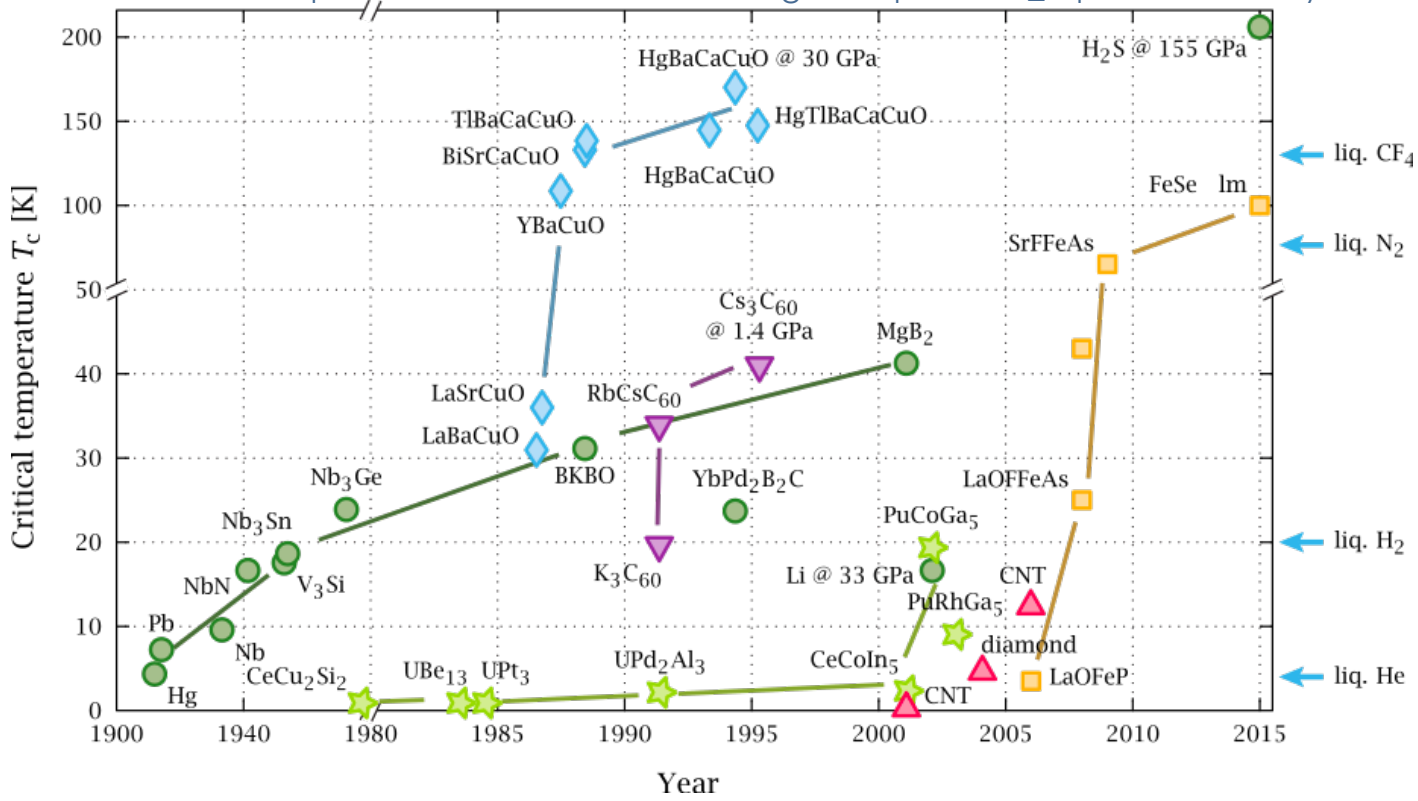


Materials progress



Kivelson & Fradkin '05

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



Conventional (BCS) superconductors

Unconventional superconductors

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

Nambu-Gorkov formalism for superconducting state

Approach 1

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

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

Green's function matrix

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

Symmetry	Δ_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

Approach 1

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

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

Cluster self-energy

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

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

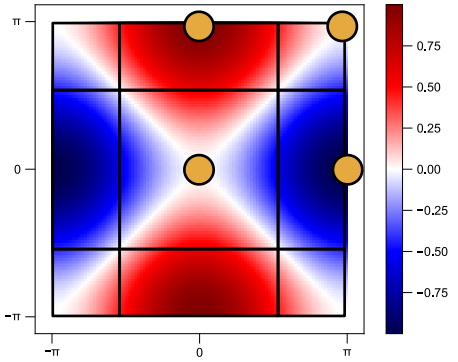
$$S[\Psi^*, \Psi] = -\int_0^\beta d\tau \int_0^\beta d\tau' \sum_{ij,\sigma} \Psi^*_{i\sigma}(\tau) \mathscr{G}_{0,ij,\sigma}(\tau - \tau') \Psi_{j\sigma}(\tau) + \frac{U}{2} \int_0^\beta d\tau \sum_i \left[\Psi^*_i(\tau)\sigma_3 \Psi_i(\tau)\right] \left[\Psi^*_i(\tau)\sigma_3 \Psi_i(\tau)\right]$$

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

(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 $\eta(\mathrm{k})$
- Switch off $\eta(\mathrm{k})$ after first (few) iterations
- Let system relax
- Calculate order parameter after convergence

Symmetry of superconducting state

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

Symmetry	Δ_k	N_c=1 (DMFT)	N_c=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	$a \sin k_x + b \sin k_y$	✘	✘
…			

DCA results for superconducting state

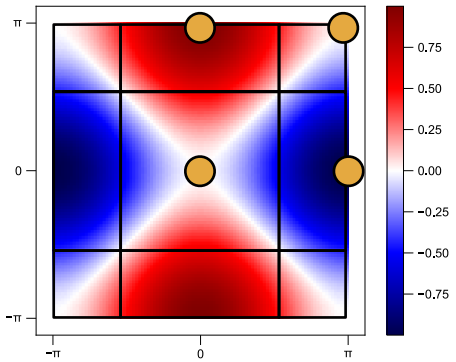
Maier et al., PRL 2000

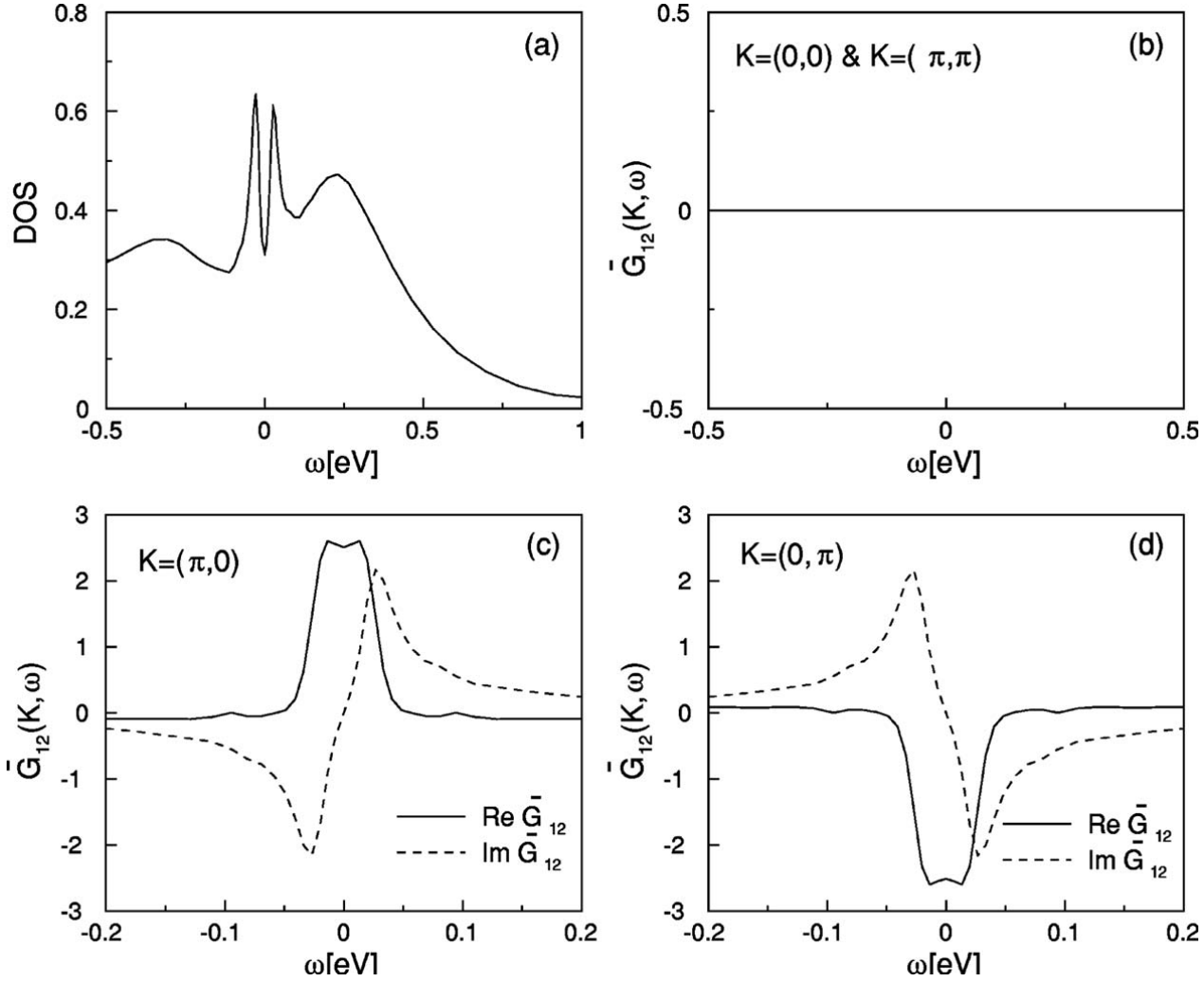
DCA (non-crossing approximation) results for SC state

- 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)





Pair-field Susceptibility

Approach 2

Definition

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

Pairing operator

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

Form-factor (d-wave)

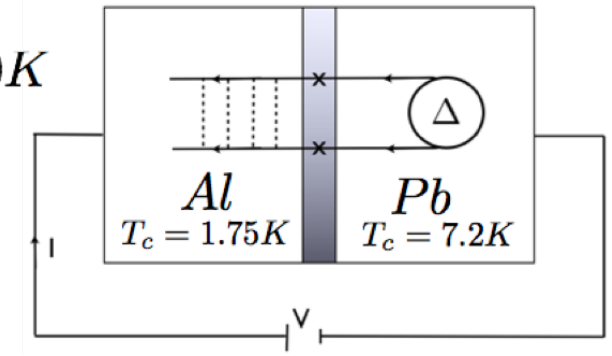
$$g_{d_{x^2-y^2}}(\mathbf{k}) = \cos k_x - \cos k_y$$

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 $T_c(S) < T < T_c(S')$

$T = 2.0K$



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

Direct calculation of response function

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

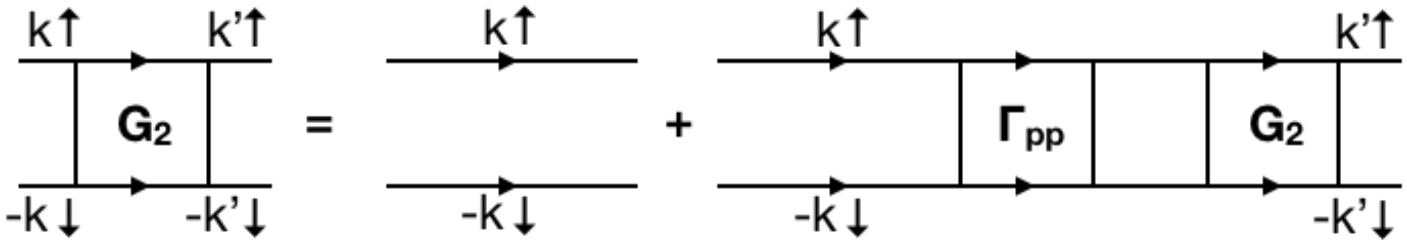
Approach 2

From 4-point 2-particle Green's function

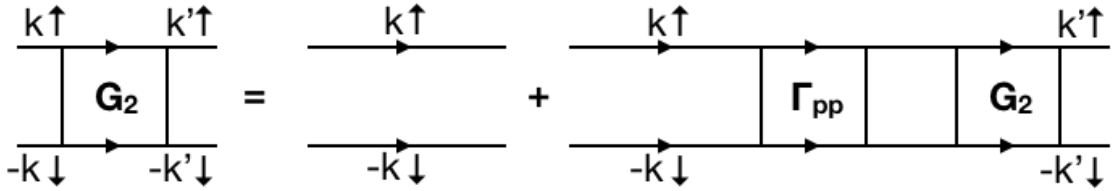
$$P_\alpha(T) = \frac{T^2}{N^2}\sum_{k,k'} g_\alpha(\mathbf{k}) G_{2,\uparrow\downarrow\downarrow\uparrow}(k,-k,-k',k') g_\alpha(\mathbf{k}')$$

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

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



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

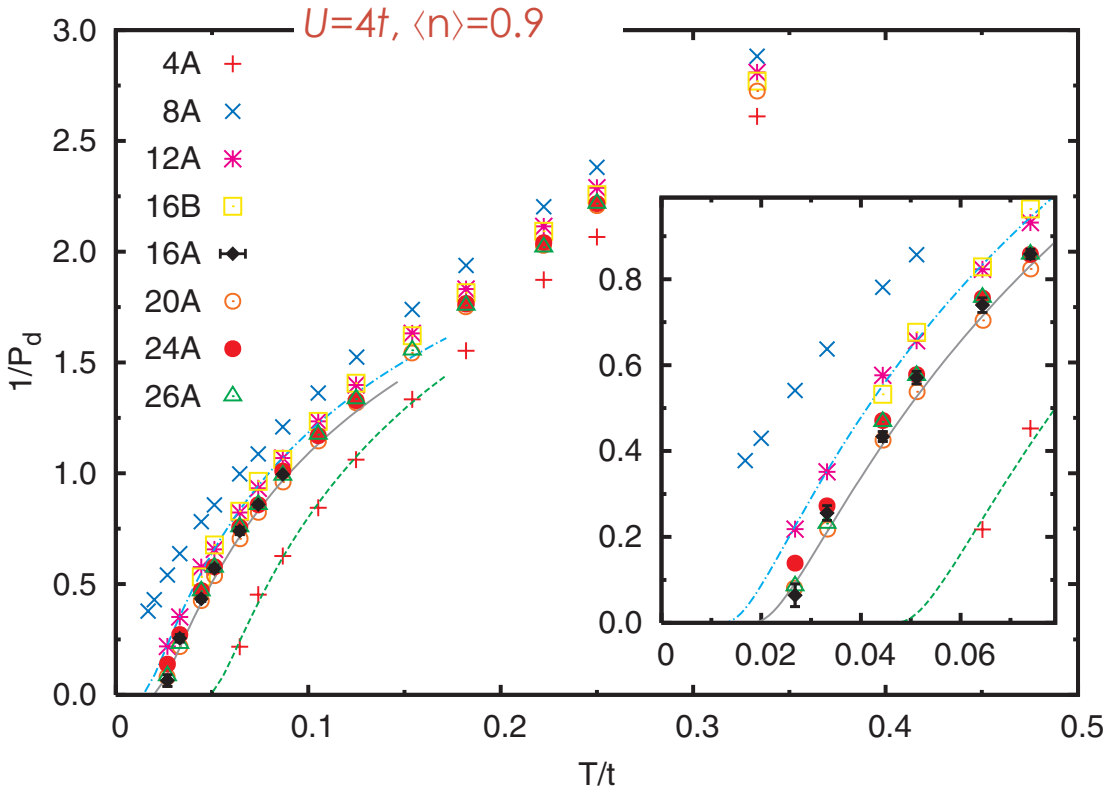
$$G_{2c,\uparrow\downarrow\downarrow\uparrow}(K,-K,-K',K') = G_{c,\uparrow}(K)G_{c,\downarrow}(-K)\delta_{K,K'} + \frac{T}{N_c}\sum_{K''} G_{c,\uparrow}(K)G_{c,\downarrow}(-K)\Gamma_{c,pp}(K,-K,-K'',K'')G_{2c,\uparrow\downarrow\downarrow\uparrow}(K'',-K'',-K',K')$$

Pairfield susceptibility

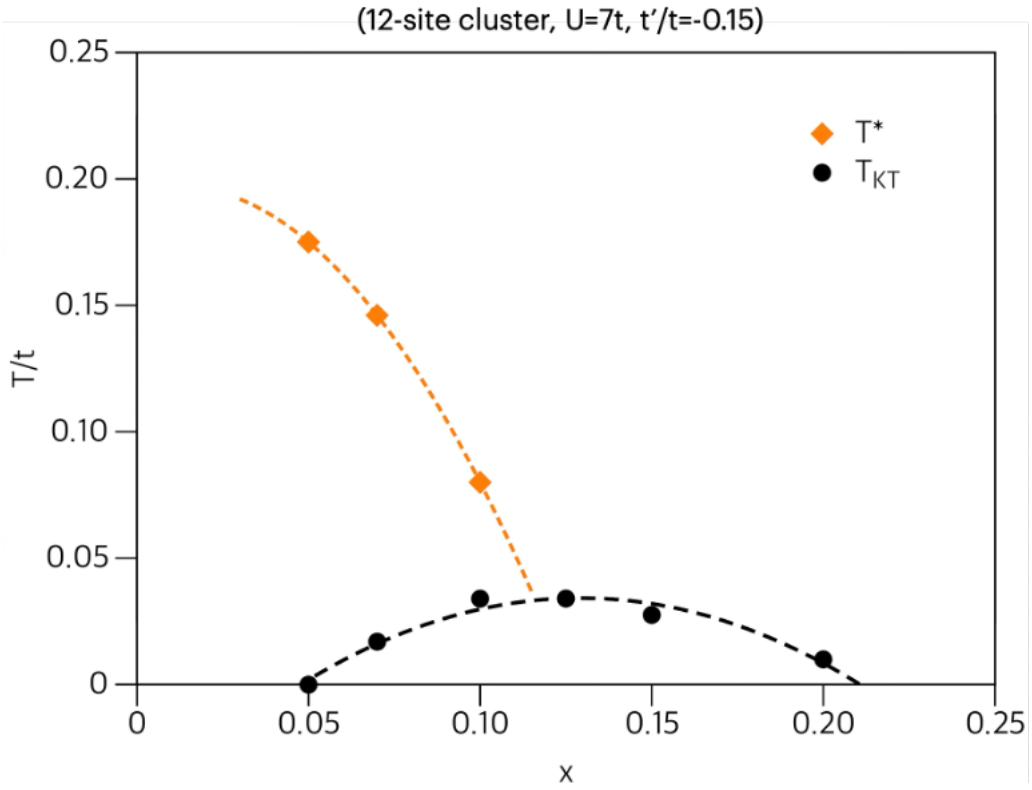
$$\longrightarrow \quad P_{\alpha}(T) = \frac{T^2}{N_c^2}\sum_{K,K'} \bar{g}_{\alpha}(\mathbf{K})\bar{G}_{2,\uparrow\downarrow\downarrow\uparrow}(K,-K,-K',K')\bar{g}_{\alpha}(\mathbf{K}')$$

Pair-field Susceptibility of 2D Hubbard model

And Phase Diagram



TAM et al., PRL '05



TAM & Scalapino, npj QM '19

Bethe-Salpeter eigenvalues and eigenfunctions

An unbiased approach

Bethe-Salpeter equation (in matrix notation)

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

"Pairing matrix" eigenvalues and eigenvectors

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

Fully renormalized version of linearized BCS gap equation

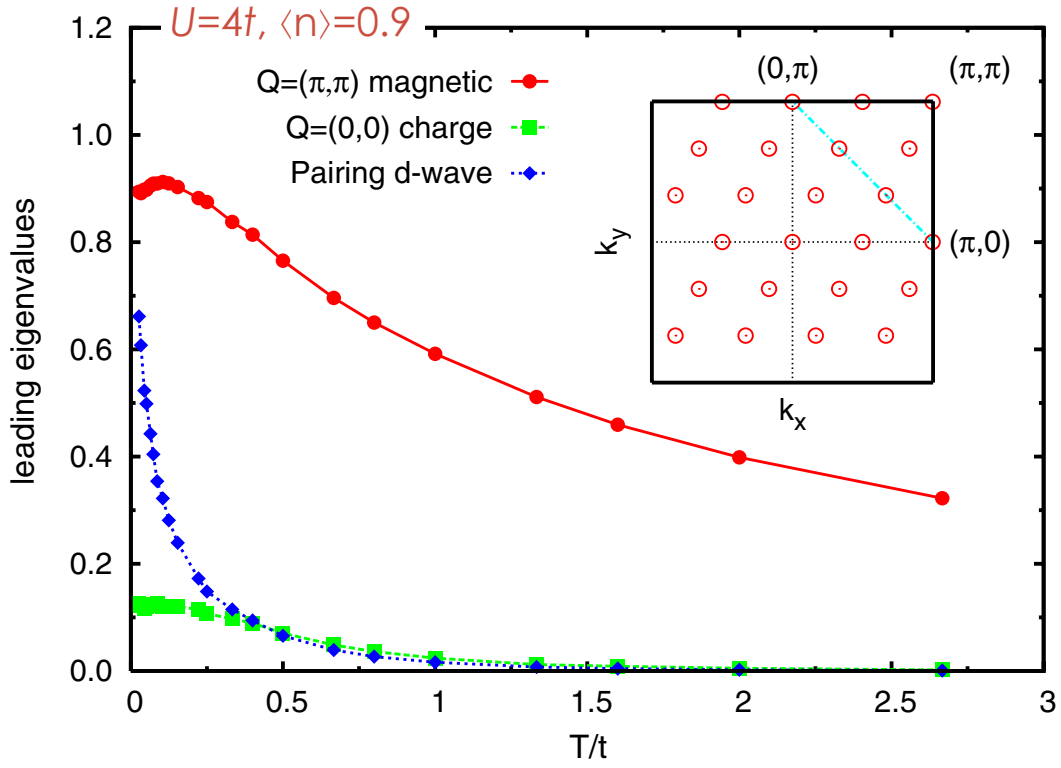
$$\longrightarrow \bar{G}_{2,\uparrow\downarrow\downarrow\uparrow}(K,K') = \bar{G}^0_{2,\uparrow\downarrow}(K)\sum_\alpha \frac{\phi^R_\alpha(K)\phi^L_\alpha(K')}{1-\lambda_\alpha}$$

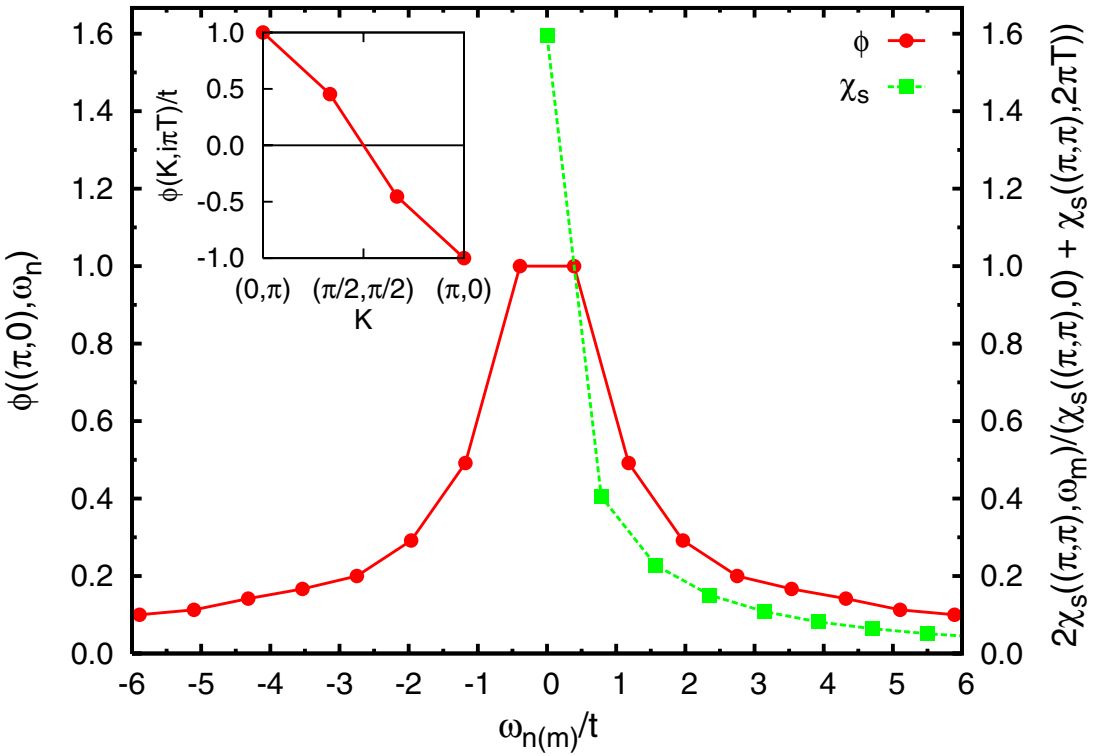
$$-\frac{1}{N}\sum_{\mathbf{k}'}\frac{V(\mathbf{k},\mathbf{k}')\tanh\left(\frac{\beta}{2}E_{\mathbf{k}'}\right)\Delta(\mathbf{k}')}{2E_{\mathbf{k}'}} = \Delta(\mathbf{k}')$$

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

Leading eigenvalues and -vectors

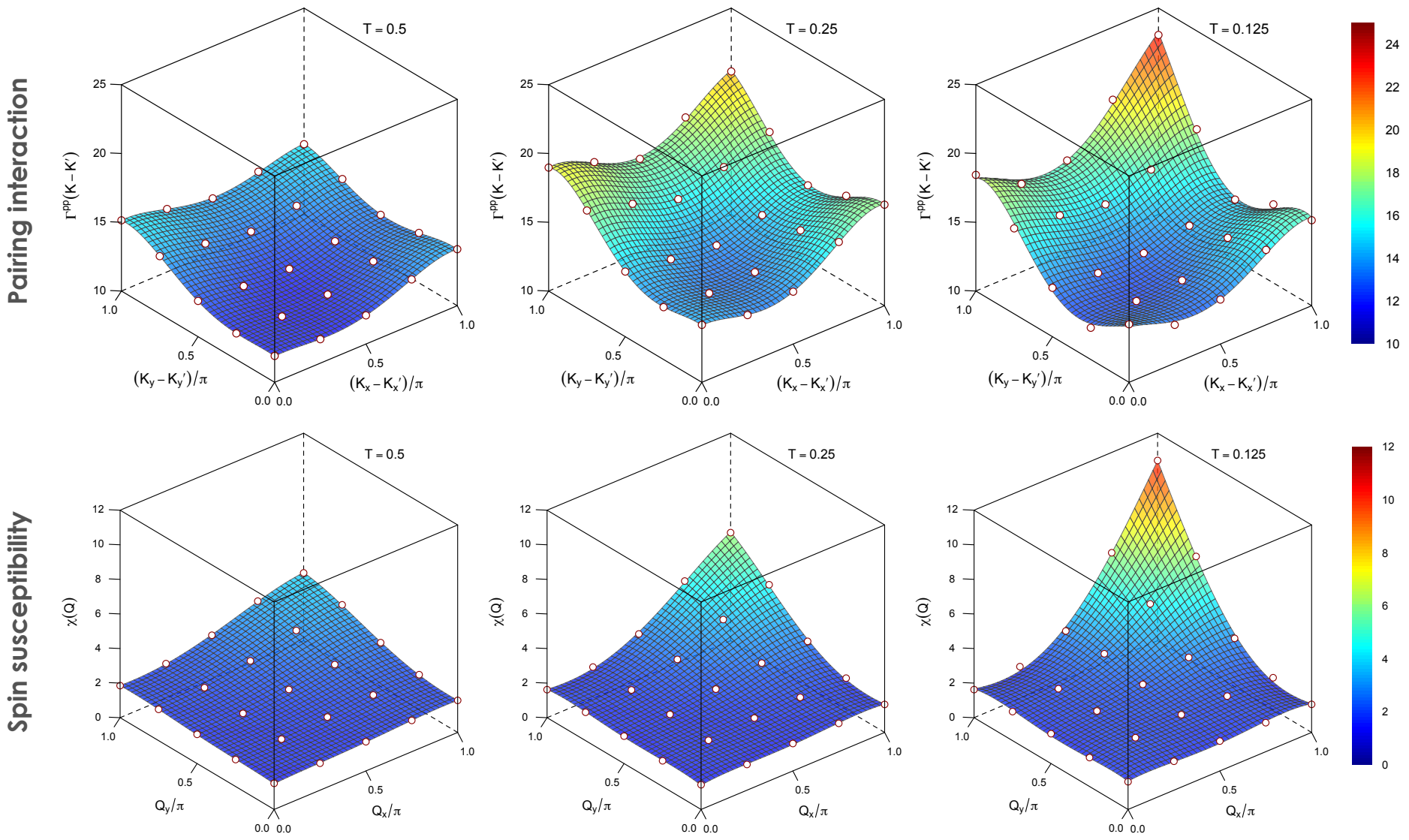
Maier et al., PRB '06





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

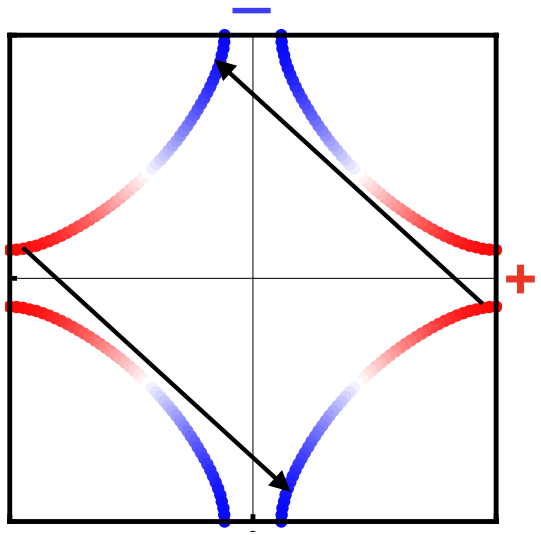
Momentum structure of pairing interaction



How does a repulsive interaction give pairing?

Momentum space

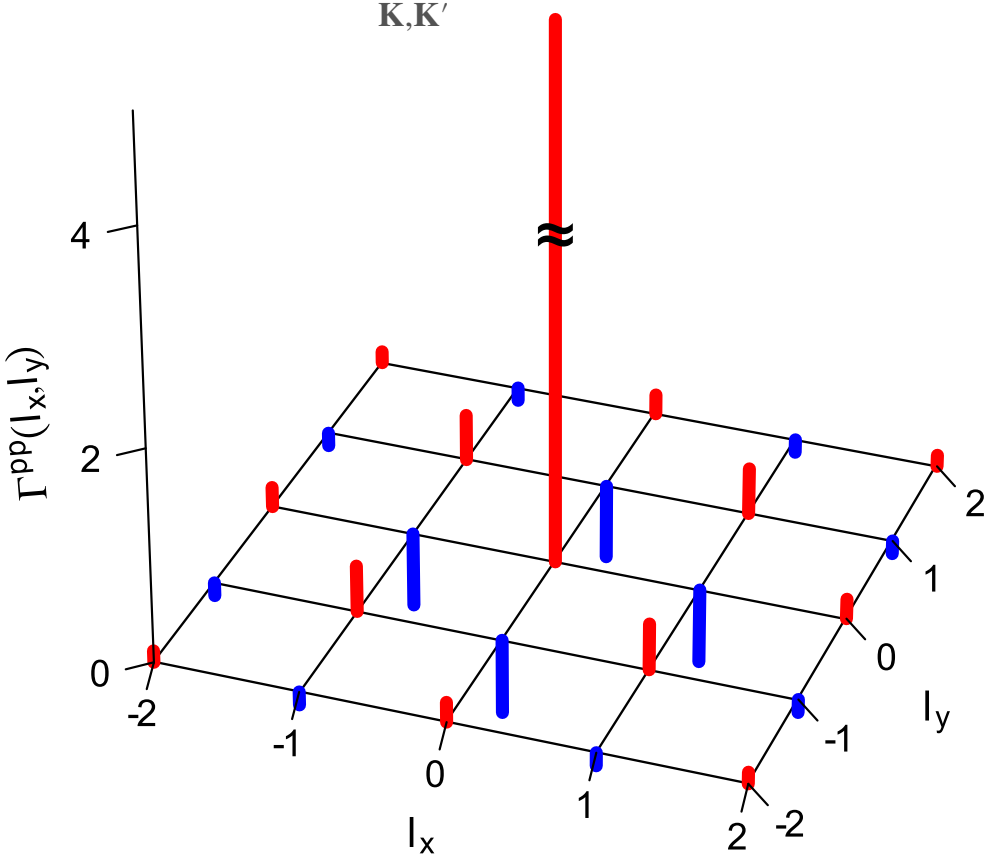
$$-\frac{T}{N_c}\sum_{K'}\Gamma_{c,pp}(K,K')\bar{G}^0_{2,\uparrow\downarrow}(K')\phi^R_\alpha(K') = \lambda_\alpha\phi^R_\alpha(K)$$



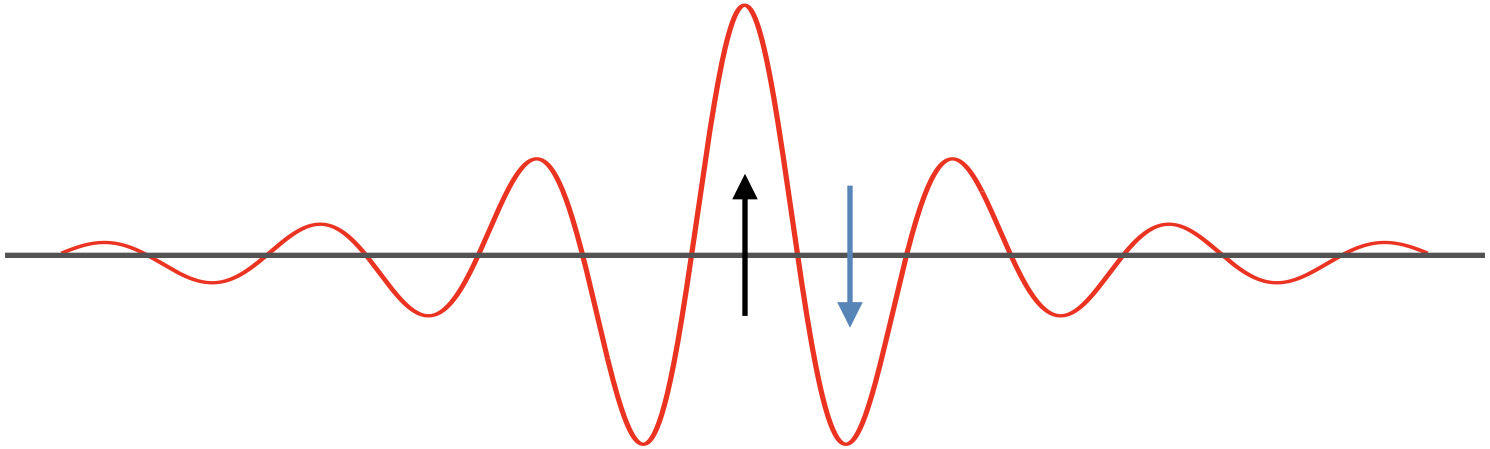
Momentum structure of pairing interaction gives rise to attractive interaction for nearest-neighbor $d_{x^2-y^2}$ pairs

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



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

Current State-of-the-Art: $La_3Ni_2O_7$

Multi-orbital Systems

Superconductivity near 80 K under > 14 GPa pressure

Bilayers are key building block

Low energy effective electronic structure captured by two-orbital bilayer Hubbard model with strong interlayer coupling:

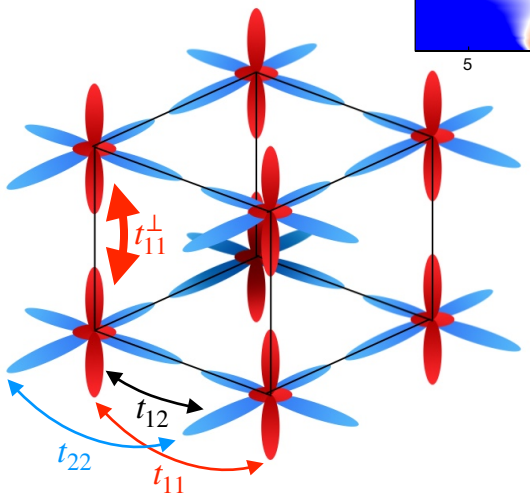
$$H = H_0 + H_{\text{int}}$$

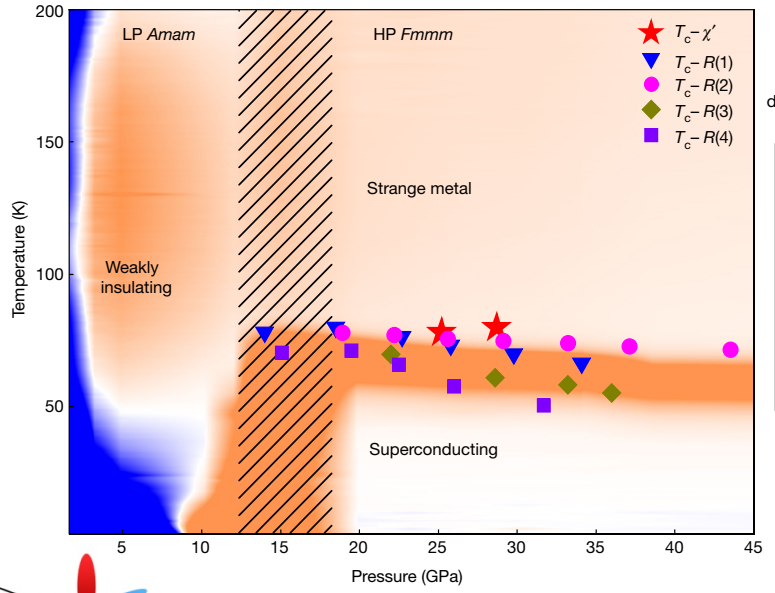
$$H_0 = \sum_{ij} \sum_{\ell\ell',\sigma} t_{ij}^{\ell\ell'} c_{i\ell\sigma}^{\dagger} c_{j\ell'\sigma}$$

$$H_{\text{int}} = U \sum_{i,\ell} n_{i\ell\uparrow} n_{i\ell\downarrow} + U' \sum_{i,\ell'<\ell} n_{i\ell} n_{i\ell'}$$

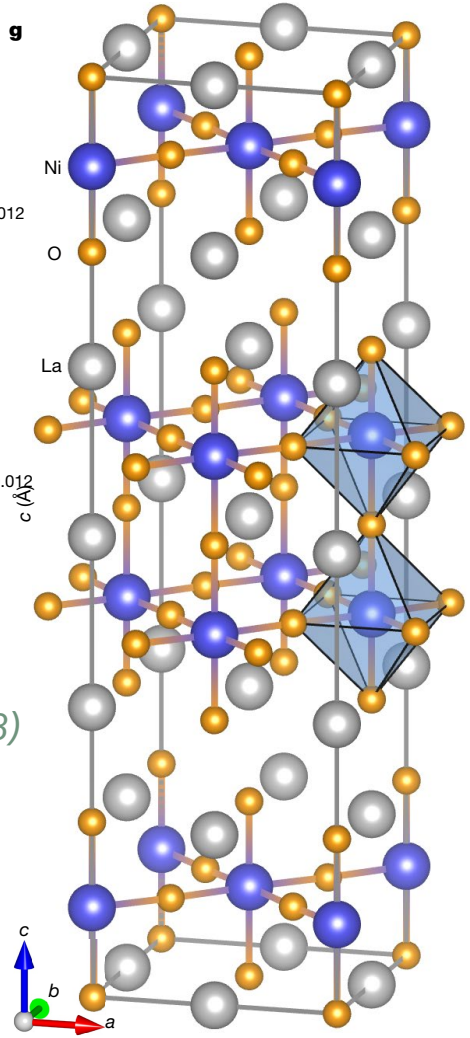
$$+J \sum_{i,\ell'<\ell} \sum_{\sigma,\sigma'} c_{i\ell\sigma}^{\dagger} c_{i\ell'\sigma'}^{\dagger} c_{i\ell\sigma'} c_{i\ell'\sigma}$$

$$+J' \sum_{i,\ell'\neq\ell} c_{i\ell\uparrow}^{\dagger} c_{i\ell\downarrow}^{\dagger} c_{i\ell'\downarrow} c_{i\ell'\uparrow}$$

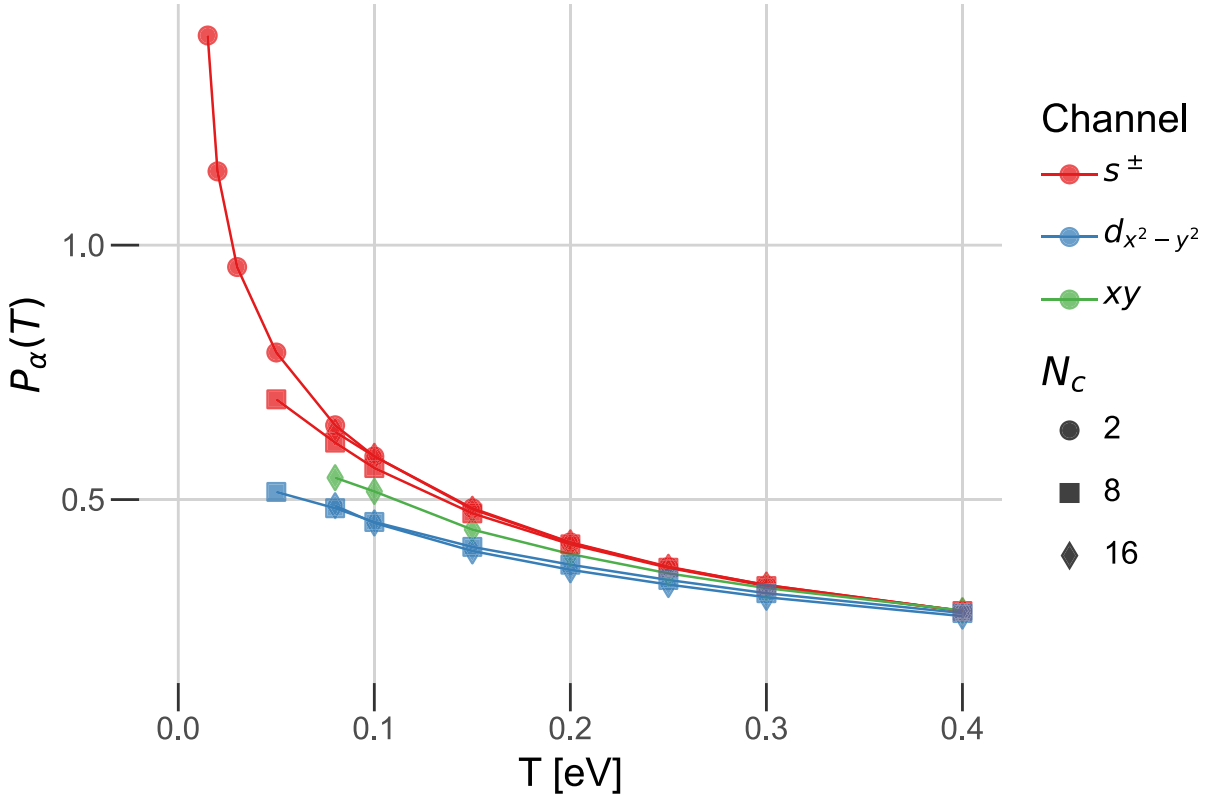


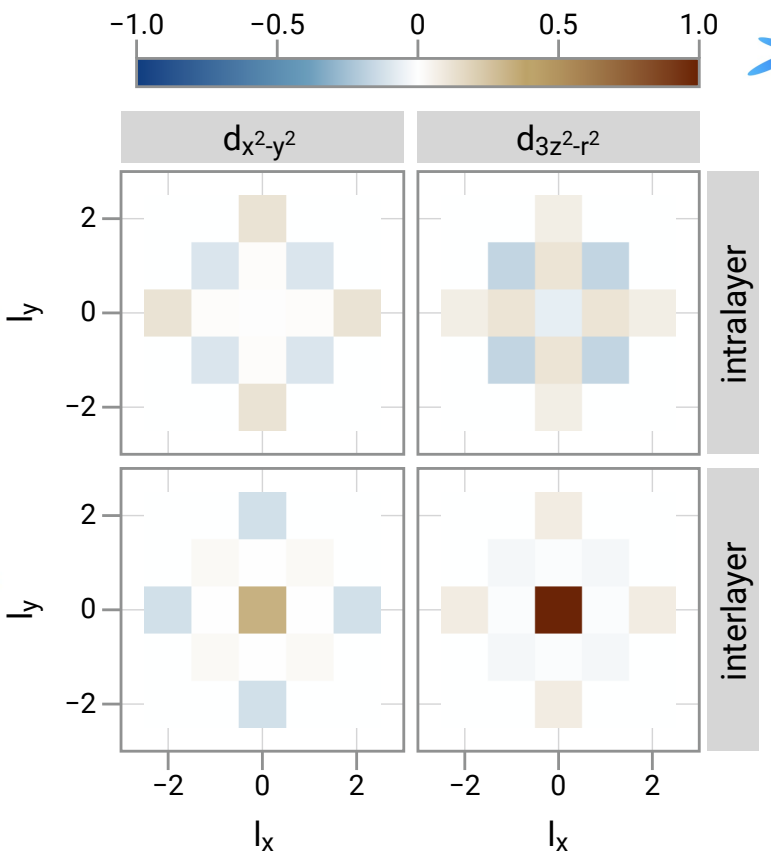


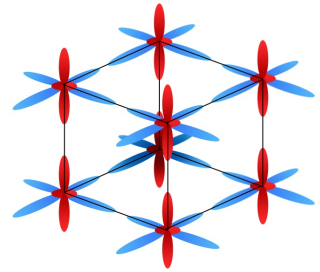
Sun et al., Nature 621, 493 (2023)



Pair-field susceptibility and leading pairing state



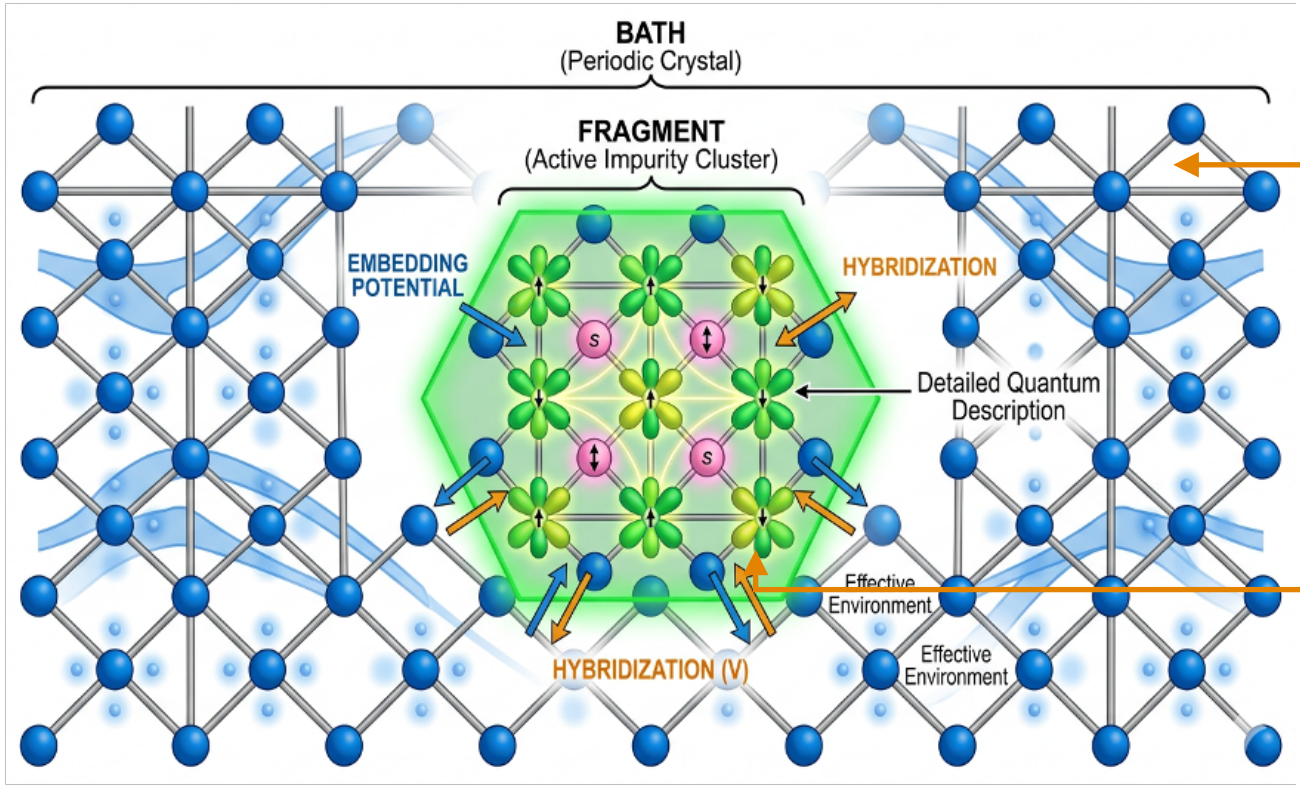




TAM et al., npj Quantum Mat. 11, 19 (2026)

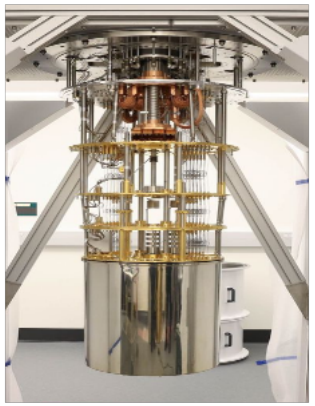
Future: Quantum Embedding on Quantum Computers

For hybrid quantum/classical materials simulations



Classical computer

Quantum computer



Bauer et al., PRX 6, 031045 (2016)
Keen et al., Quant. Sci. Tech. 5, 035001 (2020)
Vorwerk et al., Nat. Comp. Sci. 2, 424 (2022)

Quantum embedding offers a scalable and physically meaningful pathway toward quantum advantage in realistic materials simulations

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DCA++ Hands-on Session

Thomas A. Maier, June 22, 2026

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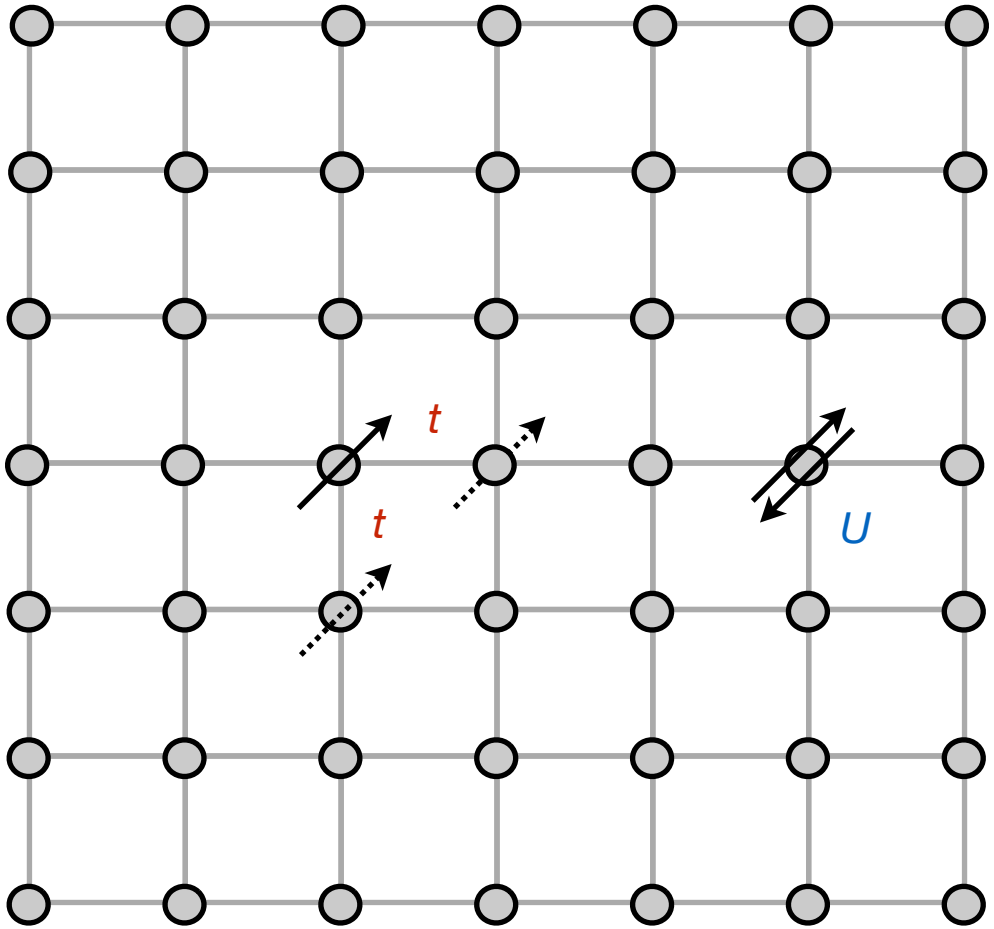
U.S. DEPARTMENT OF ENERGY

DCA++ T_c Tutorial

Calculate the superconducting transition temperature in 2D Hubbard model



DCA++ T_c Tutorial

Calculate the superconducting transition temperature in 2D Hubbard model

Prerequisites

Configure and build the application `main_dca` using the following CMake options:

```
CMAKE_BUILD_TYPE = Release
DCA_BUILD_ANALYSIS = ON
DCA_BUILD_DCA = ON
DCA_CLUSTER_SOLVER = CT-AUX
DCA_LATTICE = square
DCA_MODEL = tight-binding
DCA_POINT_GROUP = D4
DCA_RNG = std::mt19937_64  # or std::ranlux48
DCA_WITH_THREADED_SOLVER = ON
```

DCA++ T_c Tutorial

Calculate the superconducting transition temperature in 2D Hubbard model

Usage

We assume the *current working directory* to be the directory containing this file, i.e. `DCA/tutorials/tc/preconfigured`.

1. Copy the binaries `main_dca` into the current working directory.

2. Execute the `dca` job script](https://github.com/CompFUSE/DCA/blob/master/tutorials/tc/preconfigured/job.dca_U=6_d=0.95_Nc=4.sh):

```
$ ./job.dca_U=6_d=0.95_Nc=4.sh > out.dca.txt
```

Runtime on an Intel Core i7-4980HQ @ 2.8GHz (4 cores) is ~110 min.

The file `out.dca_reference.txt` provides reference output.

DCA++ T_c Tutorial

Calculate the superconducting transition temperature in 2D Hubbard model

Analysis

We will use the separate python script ‘analyzeDCA.py’ for the analysis. To use it, execute the following commands in a python shell:

```
import analyzeDCA as an

a = an.analyze("./T=0.1/dca_tp.hdf5", channel="PARTICLE_PARTICLE_UP_DOWN")

a.calcChi0Cluster()

a.buildFullChi0Lattice(nkfine=32)

a.calcG4Lattice()

a.diagonalizePPKernel()

print(a.lambdas.real[0:10])

a.plotEvecs3(0)
```

Then repeat for lower temperatures and see how leading eigenvalue grows and crosses 1.