Correlated electrons: mean-field methods and beyond

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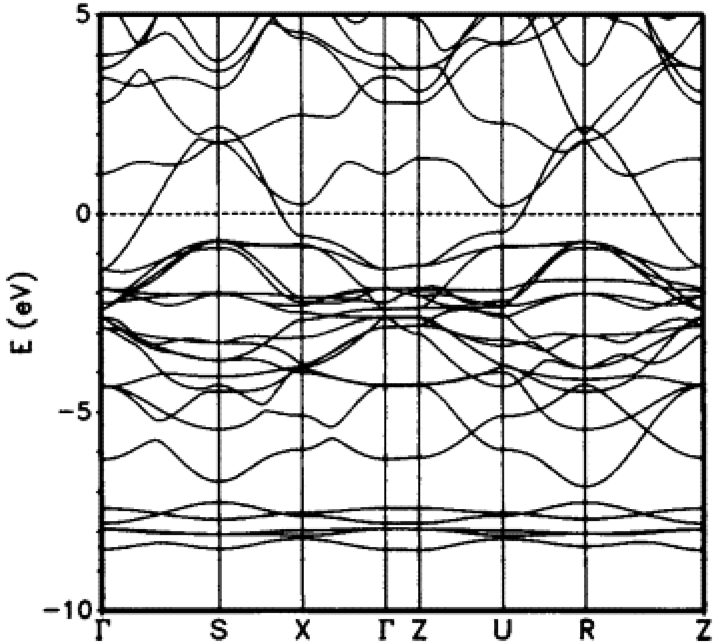
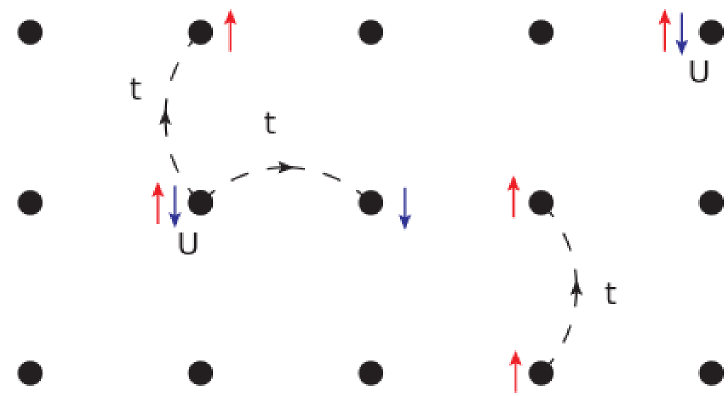
Energy scales in condensed matter physics

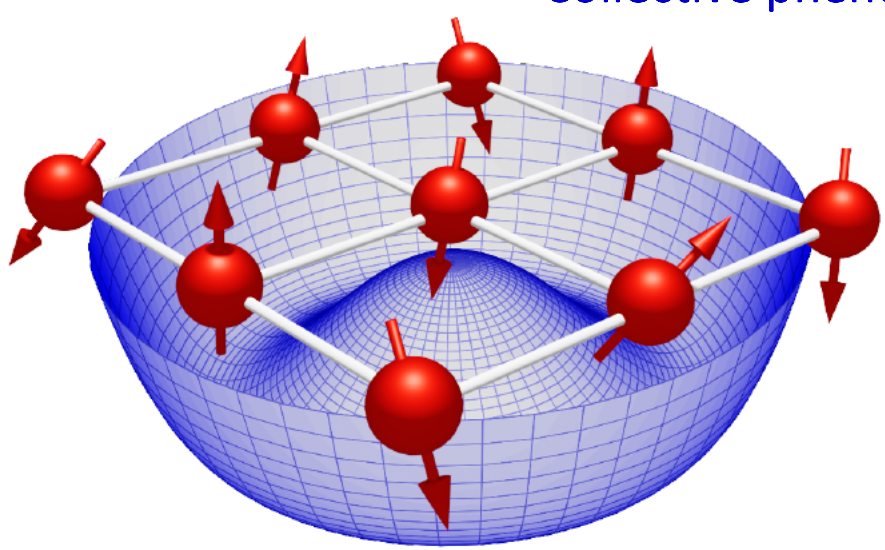
Band structure



Low-energy model



Collective phenomena



Density functional method

Hohenberg Kohn theorems

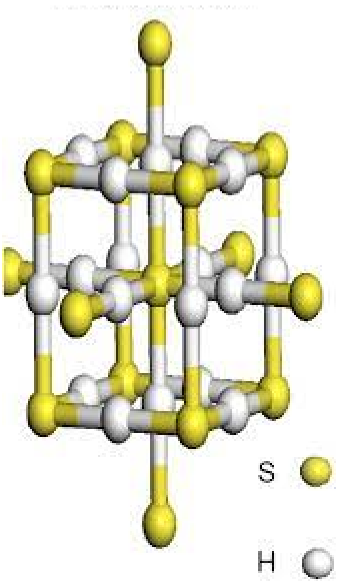
$$\hat{H} = \sum_{\mathbf{k}} \hat{n}_{\mathbf{k}} \epsilon_{\mathbf{k}} + \frac{e^2}{2} \int \frac{\hat{n}_{\mathbf{r}} \hat{n}_{\mathbf{r}'}}{|\mathbf{r} - \mathbf{r}'|} d^3r d^3r' + \int V(\mathbf{r}) \hat{n}_{\mathbf{r}} d^3r$$

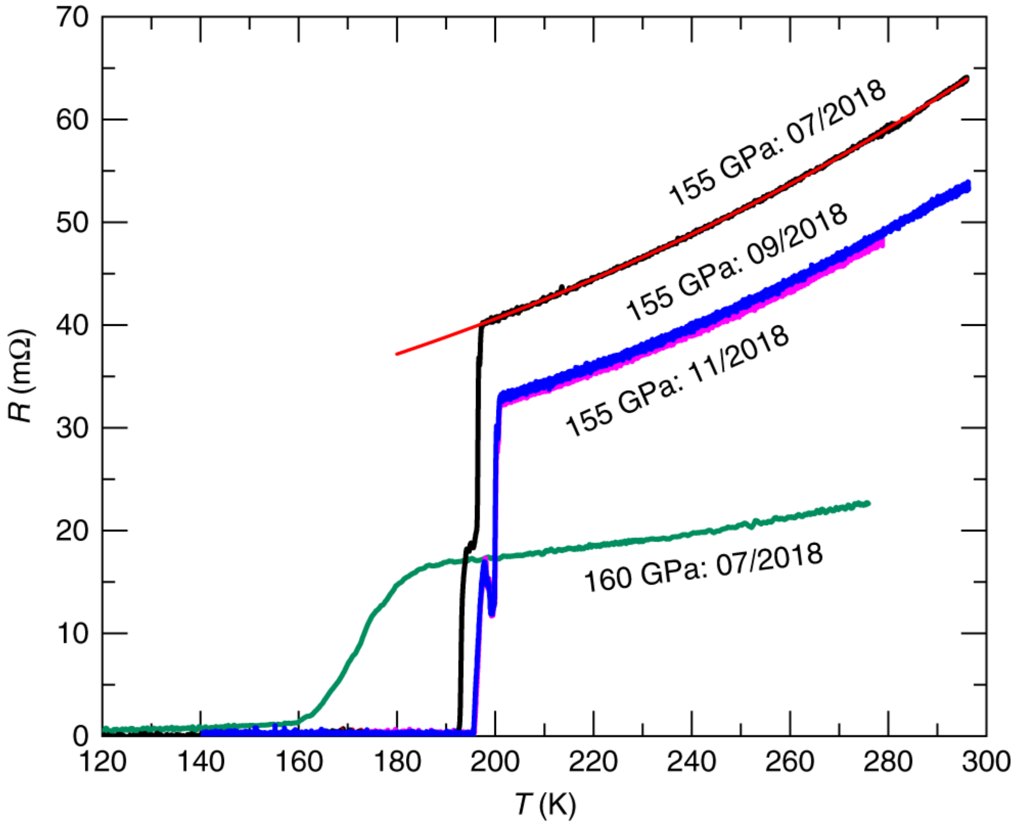
$$\hat{H}_0 = \sum_{\mathbf{k}} \hat{n}_{\mathbf{k}} \epsilon_{\mathbf{k}} + e^2 \int \frac{n_{\mathbf{r}'}}{|\mathbf{r} - \mathbf{r}'|} d^3r' \hat{n}_{\mathbf{r}} d^3r + \int \left(V(\mathbf{r}) + V^{exch}(\mathbf{r})[n_{\mathbf{r}}] \right) \hat{n}_{\mathbf{r}} d^3r$$

Local density approximation

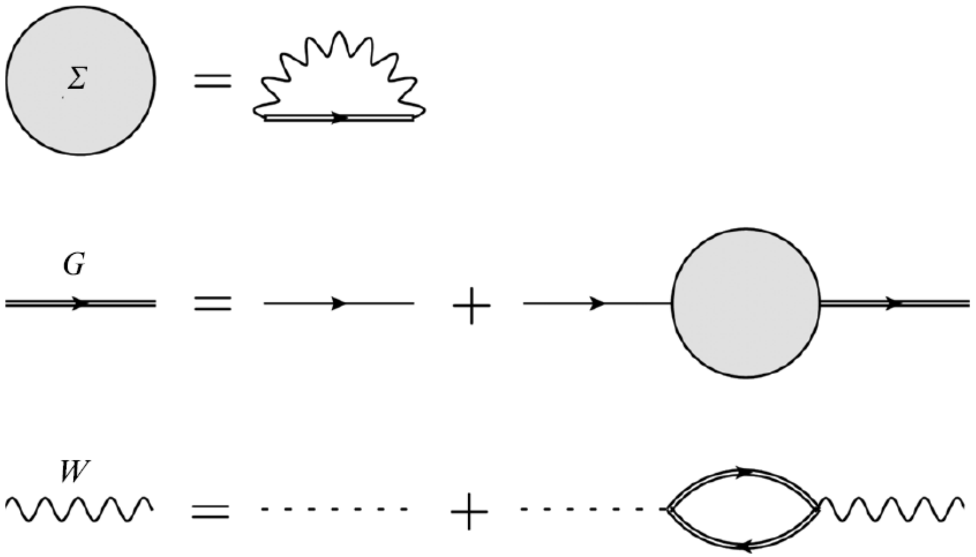
$$V^{exch}(\mathbf{r})[n_{\mathbf{r}}] \approx V^{exch}(\mathbf{r}, n_{\mathbf{r}})$$

Density functional method: H_3S superconductivity

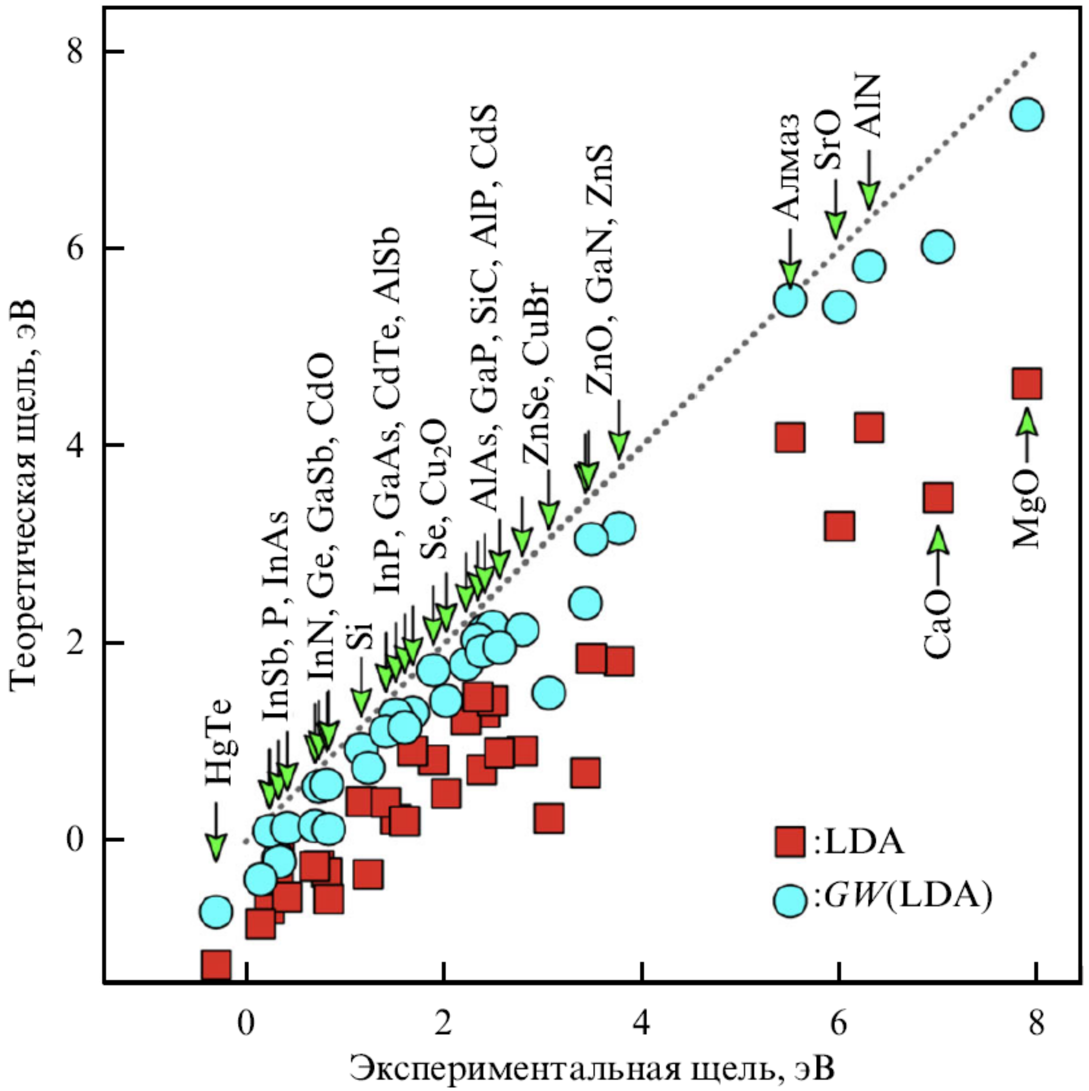




GW



GW vs LDA


Теоретическая щель, эВ
Экспериментальная щель, эВ
HgTe
InSb, P, InAs
InN, Ge, GaSb, CdO
Si
InP, GaAs, CdTe, AlSb
Se, Cu2O
AlAs, GaP, SiC, AlP, CdS
ZnSe, CuBr
ZnO, GaN, ZnS
Алмаз
SrO
AlN
CaO
MgO
:LDA
:GW(LDA)
0
2
4
6
8

Optical absorption is a two-particle phenomenon

Diamond, C, 5.5 eV

Corundum, Al_2O_3, 9.5 eV

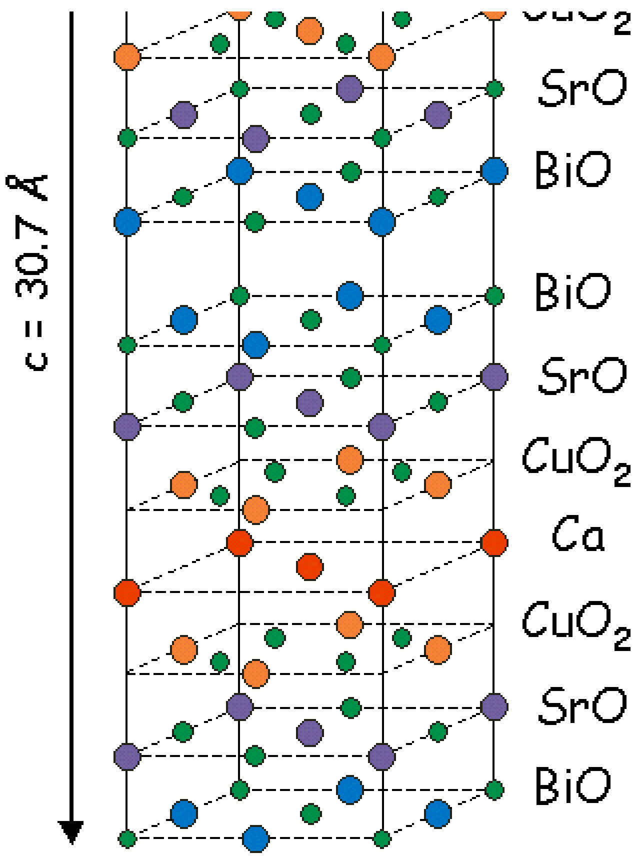
Quartz, SiO_2, 8.5 eV

Chromium oxide, Cr_2O_3, 4 eV

Nickel oxide, NiO, 4 eV

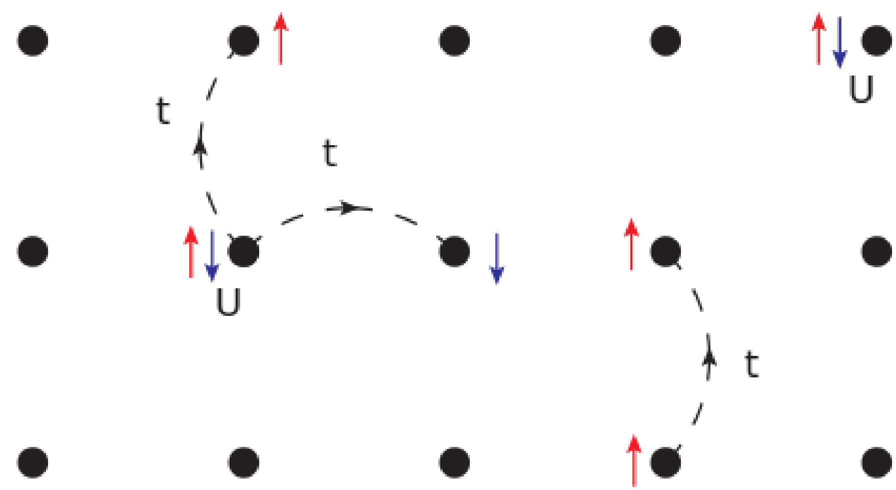
Hubbard model

$Bi_2Sr_2CaCu_2O_{8+x}$

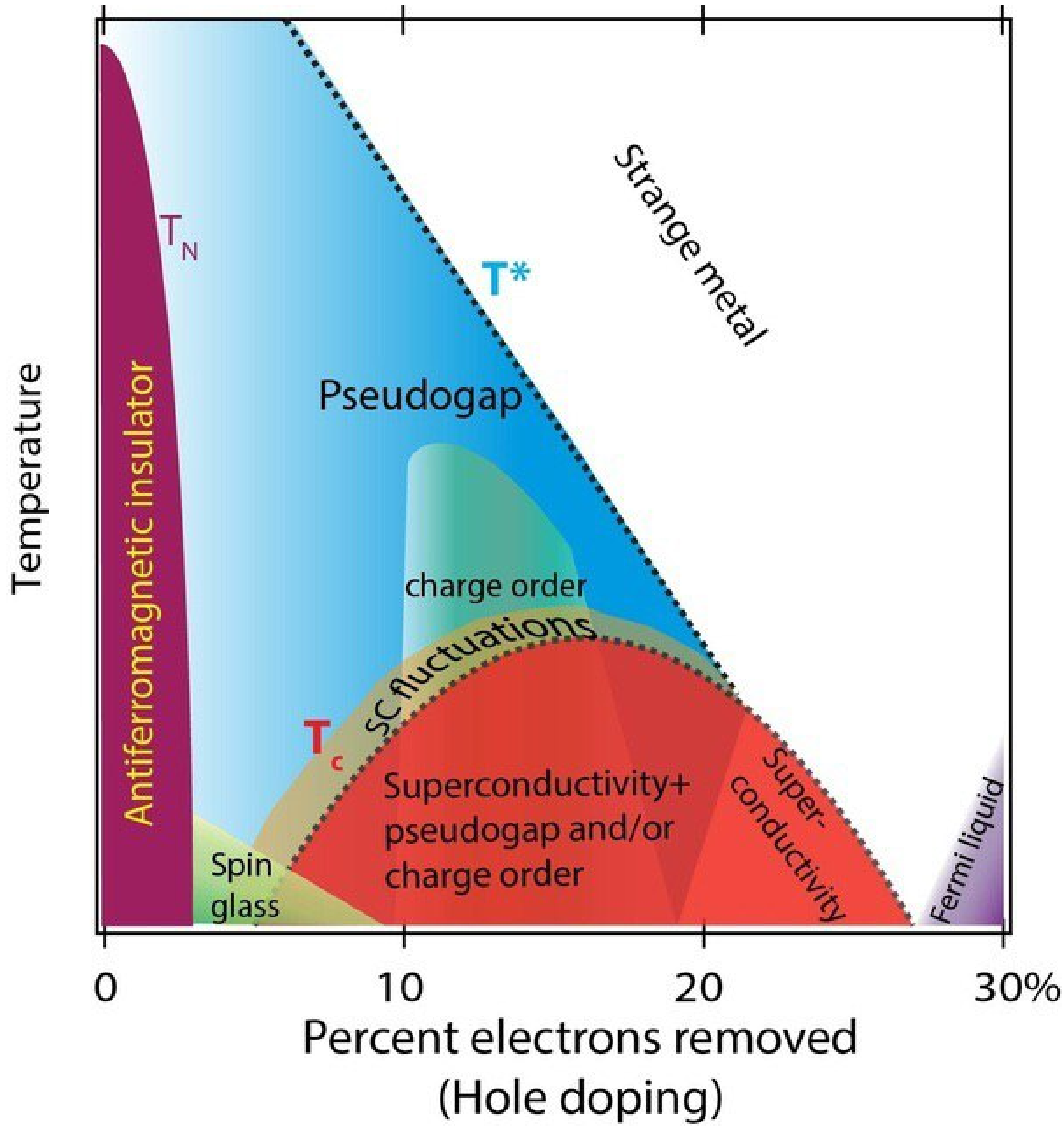


picture from
http://hoffman.physics.harvard.edu

$$H = \sum_{\langle i,j \rangle \sigma} t_{ij}\, c^\dagger_{i\sigma} c_{j\sigma} + \sum_{\langle\langle i,j \rangle\rangle \sigma} t'_{ij}\, c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$



Hubbard model: phase diagram

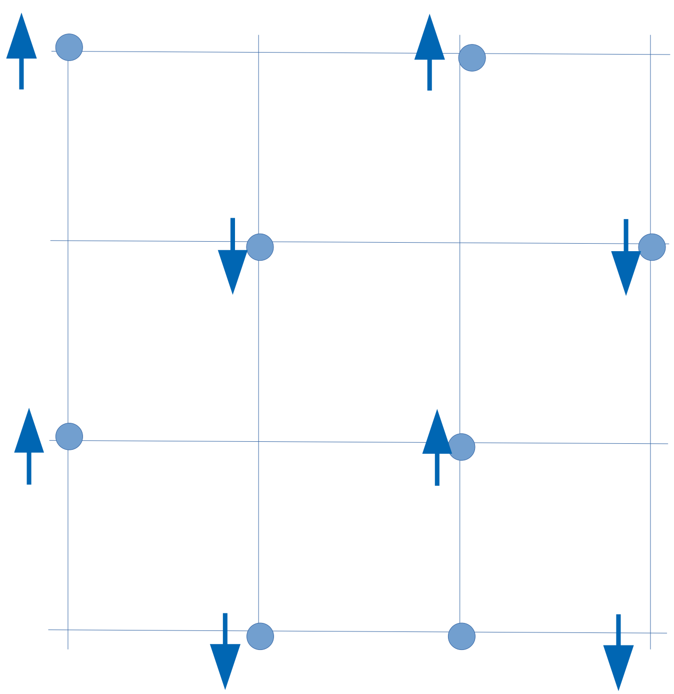


Hartree method

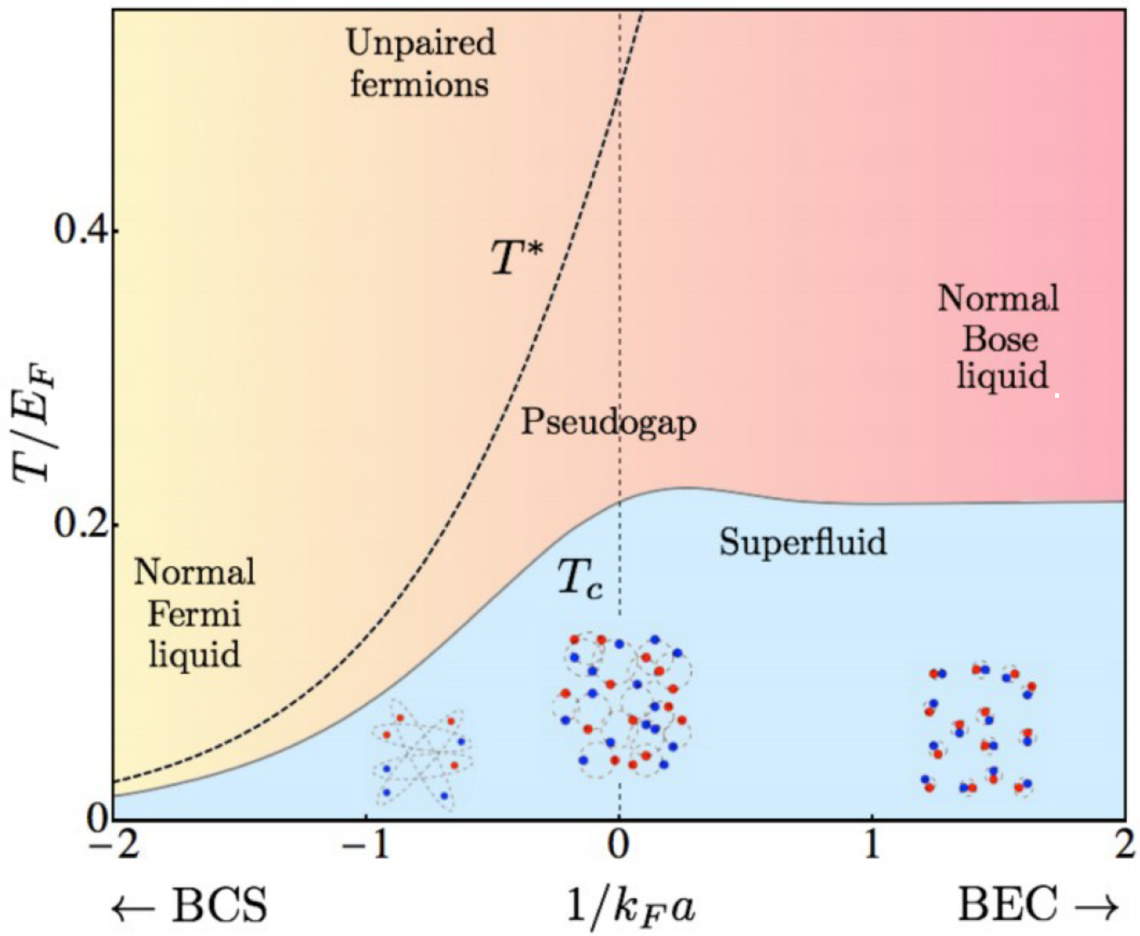
$$S = -c_1^\dagger \left(\mathcal{G}_{12}^{-1}\right) c_2 - \frac{U}{2} \sum_j \int d\tau (s^z_{\tau j})^2$$

$$S_{HF} = -c_1^\dagger \left(G_{12}^{-1}\right) c_2$$

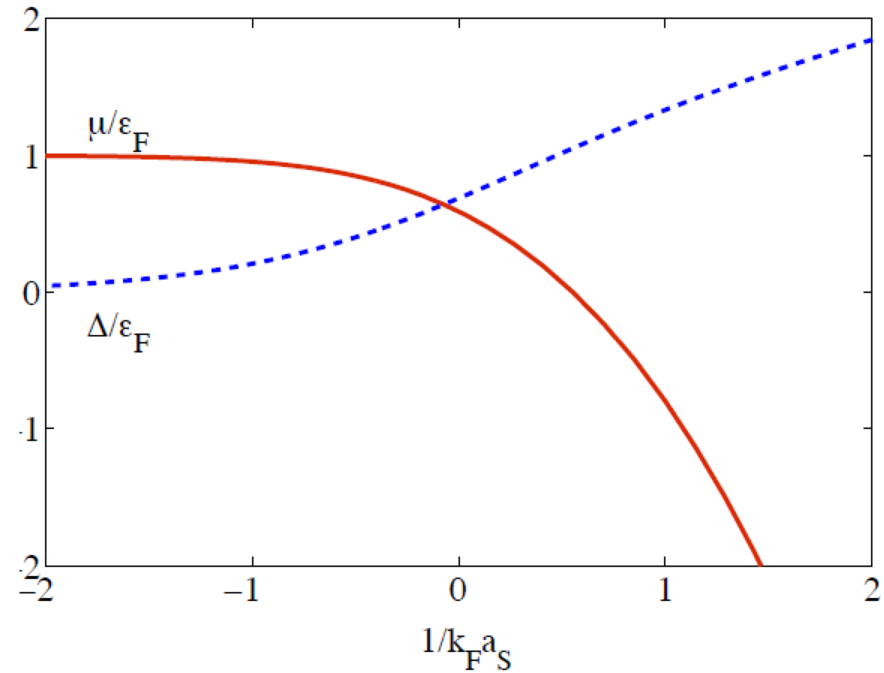
$$G^{-1} = \mathcal{G}^{-1} - \Sigma^{HF} \qquad \Sigma^{HF} = \frac{U}{2}\bar{s}$$



BEC-BCS crossover



BCS BEC Crossover - Randeria, Taylor, 2014



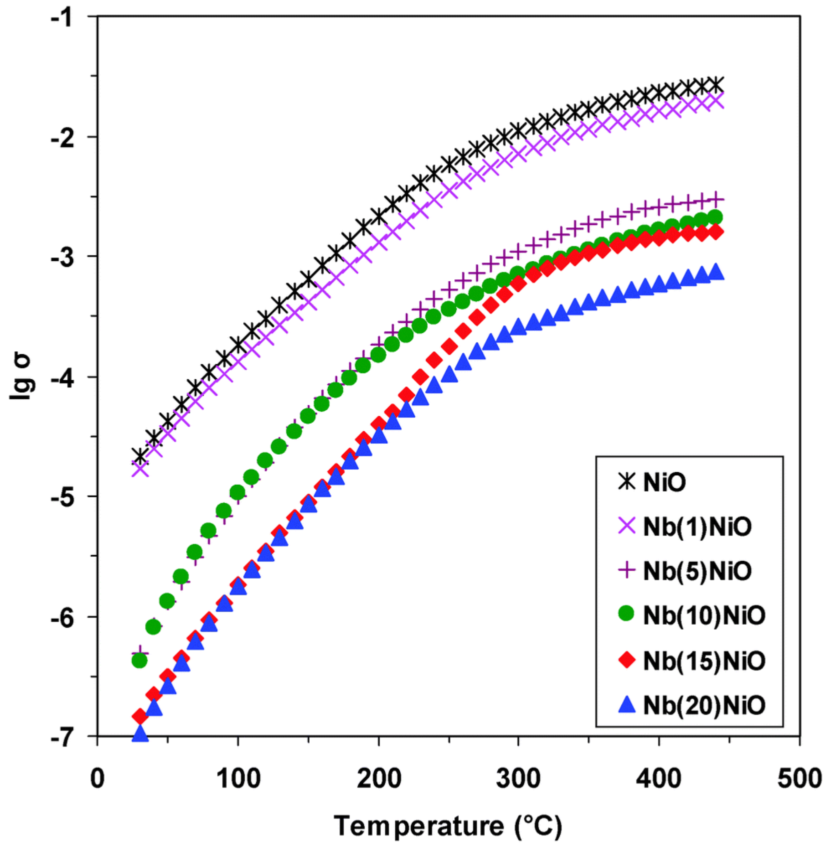
$$\Delta \equiv \frac{U}{V}\sum_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}} = -\frac{U}{V}\sum_{\mathbf{k}} \frac{\Delta}{2E_{\mathbf{k}}}$$

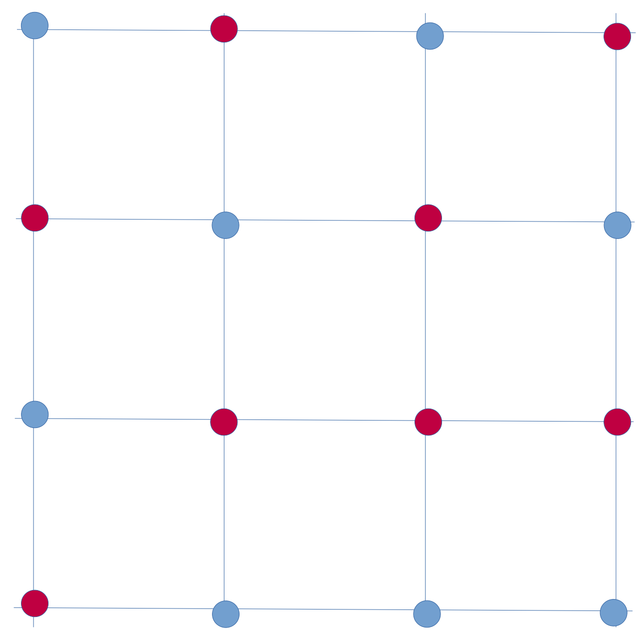
$$n = \frac{1}{V}\sum_{\mathbf{k}} v_{\mathbf{k}}^2 = \frac{1}{2V}\sum_{\mathbf{k}} \left(1 - \frac{\epsilon_{\mathbf{k}} - \mu}{E_{\mathbf{k}}}\right)$$

$$E_{\mathbf{k}} = \sqrt{(\epsilon_{\mathbf{k}} - \mu)^2 + \Delta^2}$$

Mott insulators

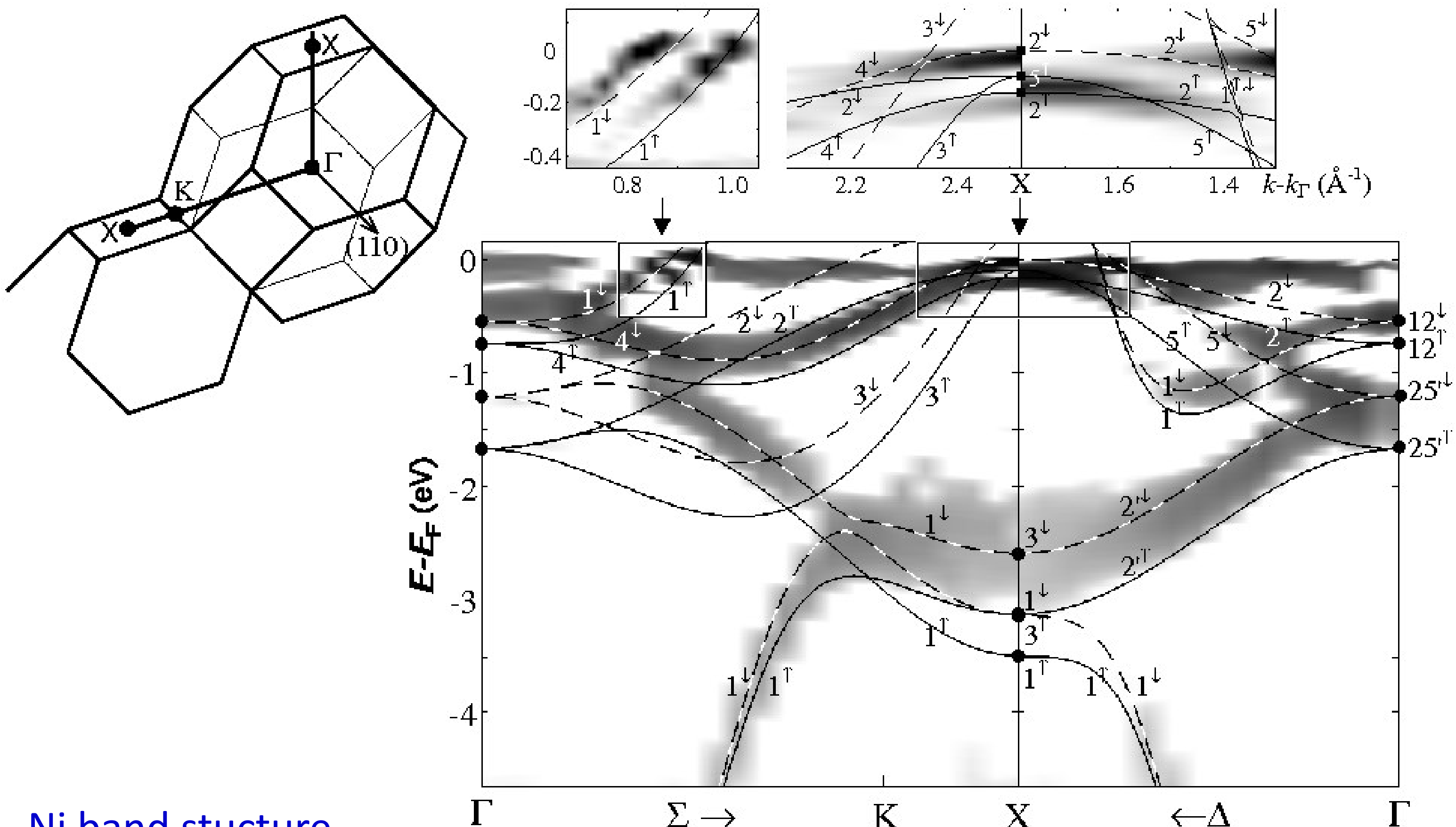
$$Ni^{2+}O^{2-} + Ni^{2+}O^{2-} \leftrightarrow Ni^{+}O^{2-} + Ni^{3+}O^{2-}$$





Gutzwiller method

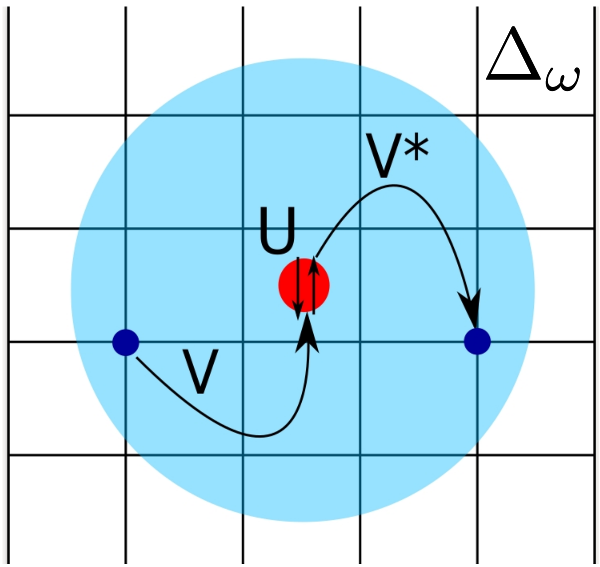
$$|\Psi\rangle = \Pi_j (1 - \alpha c^\dagger_{j\uparrow} c^\dagger_{j\downarrow}) |\Psi_0\rangle$$

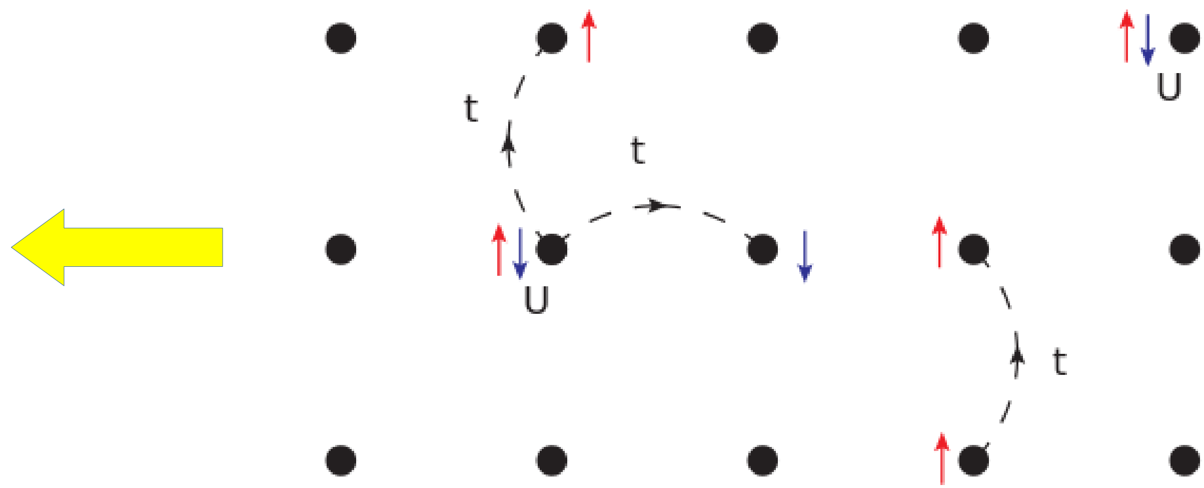


Ni band stucture

Credits: Bünemann, J et al. Europhysics Letters 61: 667 (2003)

$$S = S_{at}[c^\dagger, c] + \iint_0^\beta \Delta_{\tau-\tau'} c^\dagger_\tau, c_{\tau'} d\tau d\tau'$$





DMFT: the simplest derivation

$$S = \sum_j S_{at}[c_j, c_j^\dagger] + \sum_{k\omega} \epsilon_k c_{k\omega}^\dagger c_{k\omega}$$

$$S_{imp}[c_j, c_j^\dagger] = S_{at}[c_j, c_j^\dagger] + \sum_\omega \Delta_\omega c_\omega^\dagger c_\omega$$

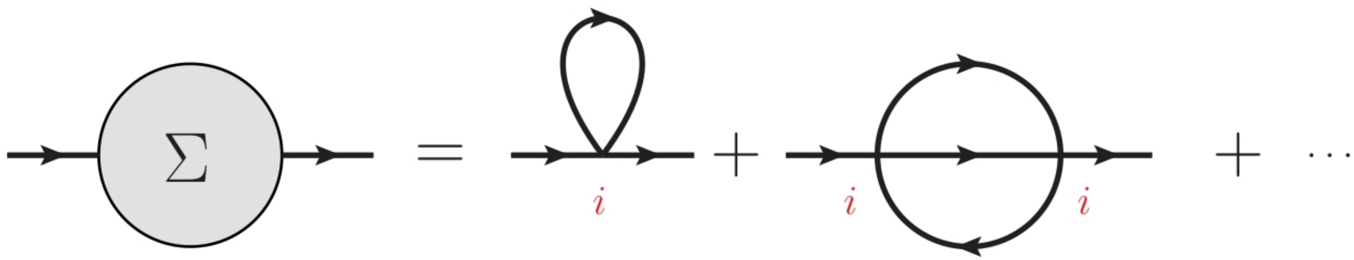
$$S = \sum_j S_{imp}[c_j, c_j^\dagger] + \sum_{k\omega} (\epsilon_k - \Delta_\omega) c_{k\omega}^\dagger c_{k\omega}$$

$$\tilde{S}_{imp}[c_j, c_j^\dagger] = -\sum_\omega c_{j\omega}^\dagger \mathcal{G}_\omega^{-1} c_{j\omega}$$

$$G = \frac{1}{\mathcal{G}_\omega^{-1} + \Delta_\omega - \epsilon_k} = \frac{1}{i\omega - \varepsilon_k - \Sigma_\omega}$$

$$\mathcal{G}_\omega = \frac{1}{N} \sum_k G_{k\omega}$$

DMFT: diagram formulation



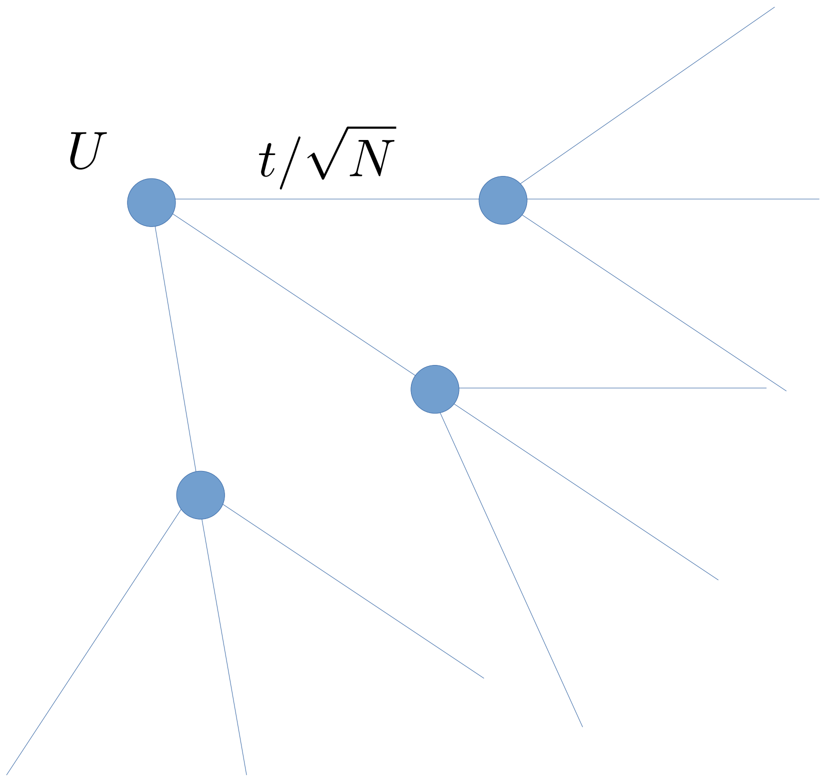
$$G^{(0)} = \frac{1}{\omega - \varepsilon_k - \Sigma_\omega}$$

The main physical effect in Fermi-liquid state is the DOS renormalization

$$G^{(0)}_{\omega\to 0} = \frac{Z}{\omega - Z\varepsilon_k}, \quad Z = \frac{1}{1 - \partial_\omega \Sigma_{\omega\to 0}}$$

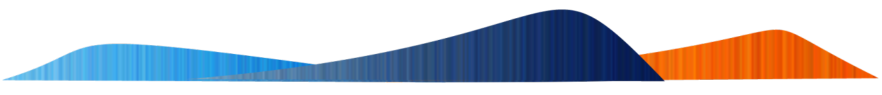
DMFT: infinite coordination number limit

Bethe lattice



$$\Delta_\omega = t^2 G_\omega$$

$$\text{corrections} \propto 1/N$$



Impurity problem: continuous-time QMC solvers

$$S = -G_0^{-1} \sum_{\omega s} c^{\dagger}_{\omega s} c_{\omega s} + U \int_0^{\beta} n_{\tau\uparrow} n_{\tau\downarrow} d\tau$$

W

Electron-hole transformation $n_{\downarrow} \to (1 - \tilde{n}_{\downarrow})$ makes the interation attractive.

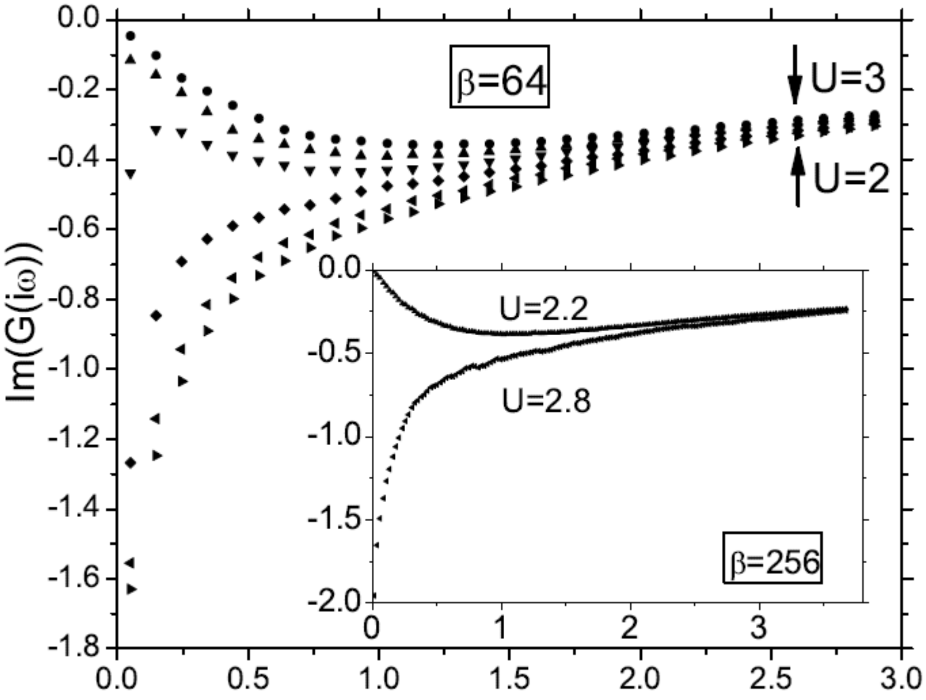
$$T e^{-\int W^0(\tau) d\tau} = 1 + U \int n^0_{\uparrow}(\tau) n^0_{\downarrow}(\tau) d\tau + \frac{1}{2!} U^2 T \int \int n^0_{\uparrow}(\tau_1) n^0_{\downarrow}(\tau_1) n^0_{\uparrow}(\tau_2) n^0_{\downarrow}(\tau_2) d\tau d\tau' + \ldots$$

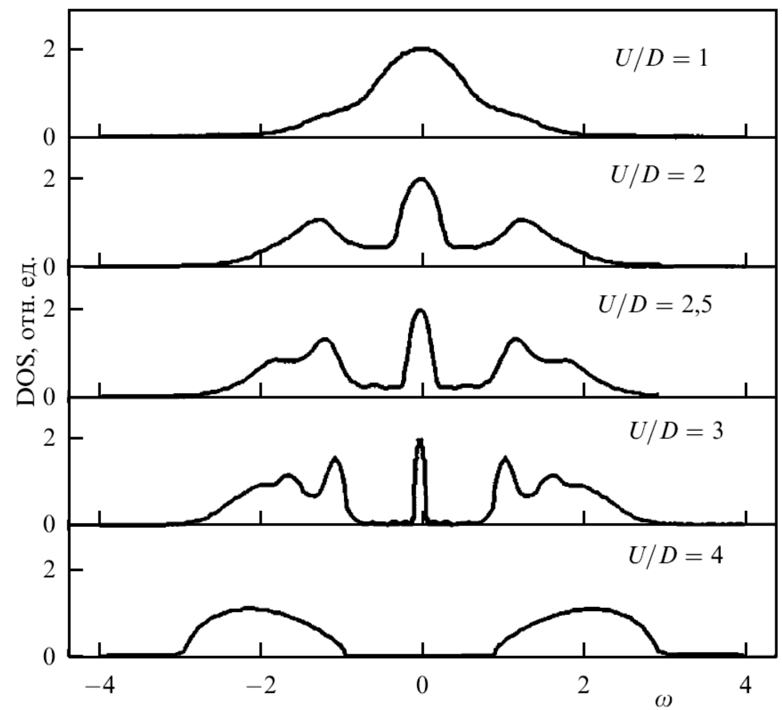
The series always converges for a finite fermionic system at finite temperature.

We perform a random walk in the space of {k, (arguments of integration)}

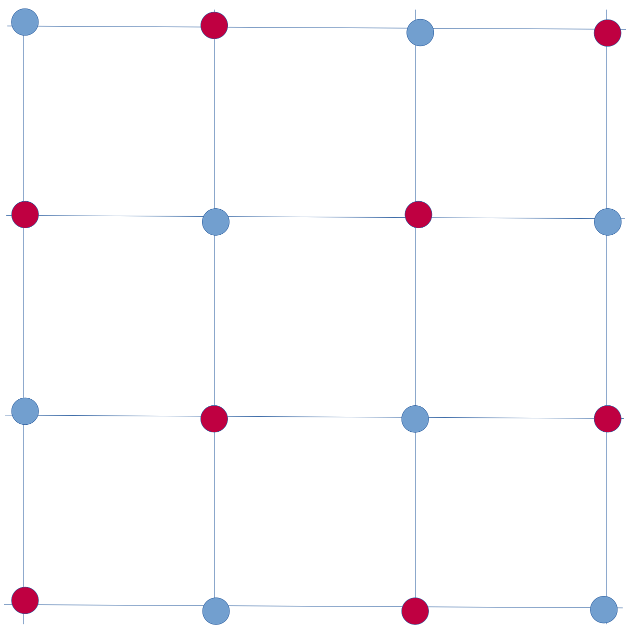
A.R., V. V. Savkin, and A. I. Lichtenstein,
Phys. Rev. B 72 035122 (2005).

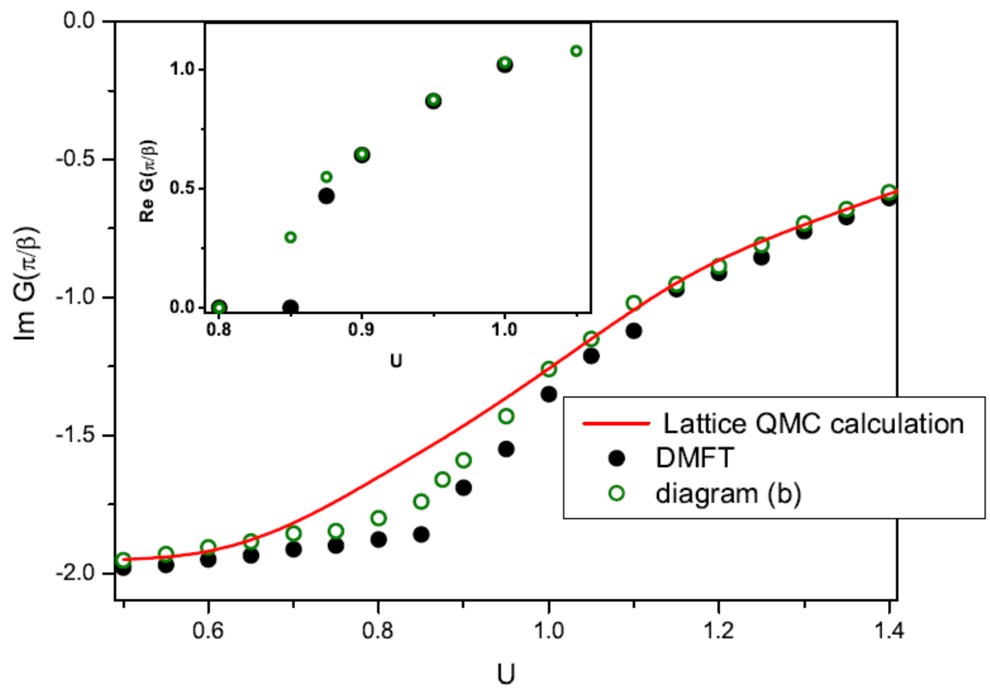
DMFT: Mott transition





DMFT: AF ordering





DMFT: neutron matter

$$G = \frac{1}{\mathcal{G}_\omega^{-1} + \Delta_\omega - \epsilon_k} \qquad \mathcal{G}_\omega = \int_{k<k_D} G_{k\omega} d^3$$

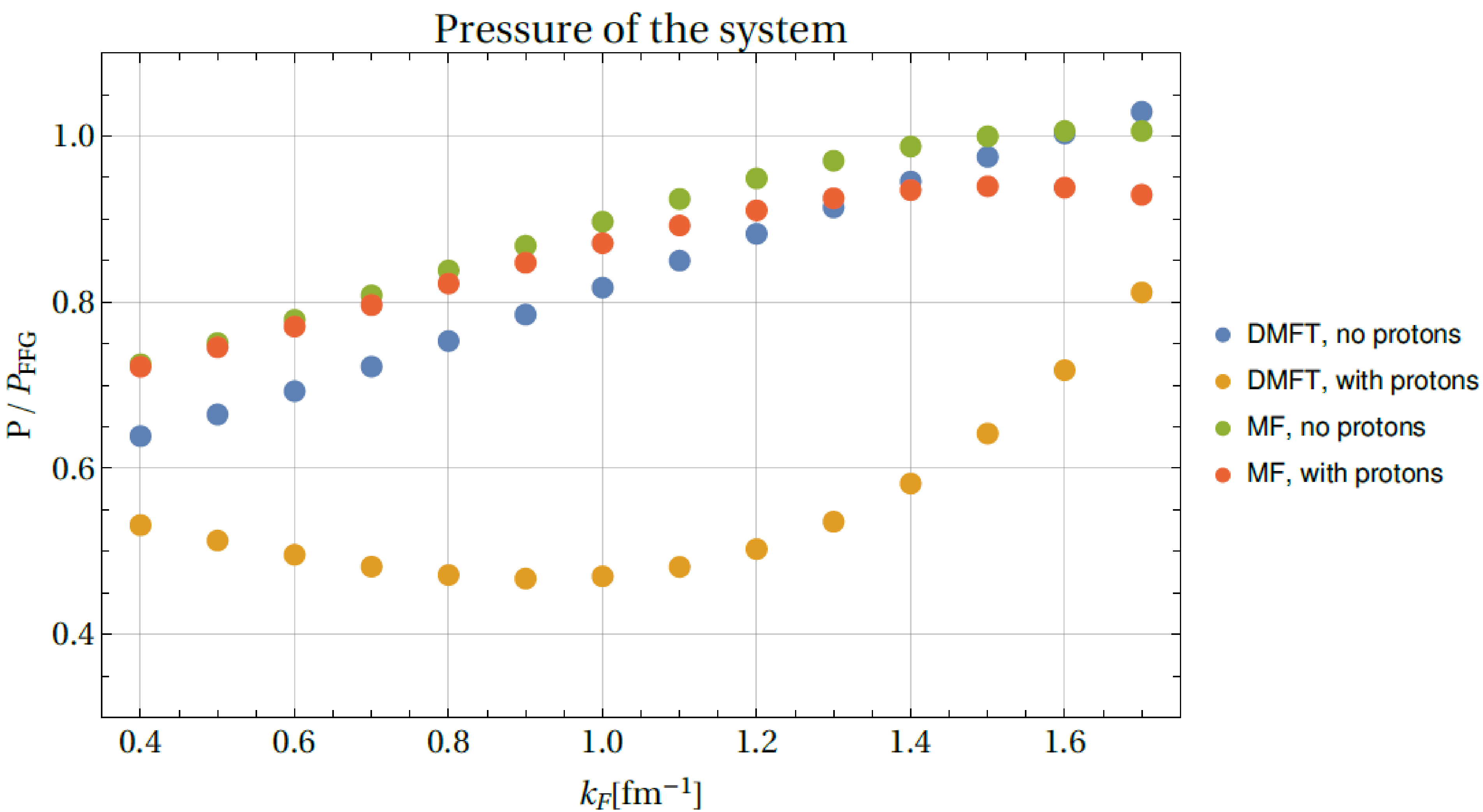
$$S^{AIM}[c_j^\dagger, c_j] = \sum_{l,s,\omega} c_{j\omega ls}^\dagger(-i\omega + \Delta_l(i\omega))c_{j\omega ls} + \frac{1}{2}\sum_{l,s,\omega} \tilde{\Delta}_{\omega l}(c_{j\omega ls}^\dagger c_{j\omega l\bar{s}}^\dagger + c_{j\omega ls}c_{j\omega l\bar{s}}) + S^{int}[c_j^\dagger, c_j]$$

$$\Delta(i\omega) \xrightarrow{\text{AIM solver}} G_{imp}(i\omega)$$

$$\Sigma_{imp}(i\omega) = (i\omega + \mu - \Delta(i\omega)) - G_{imp}^{-1}(i\omega)$$

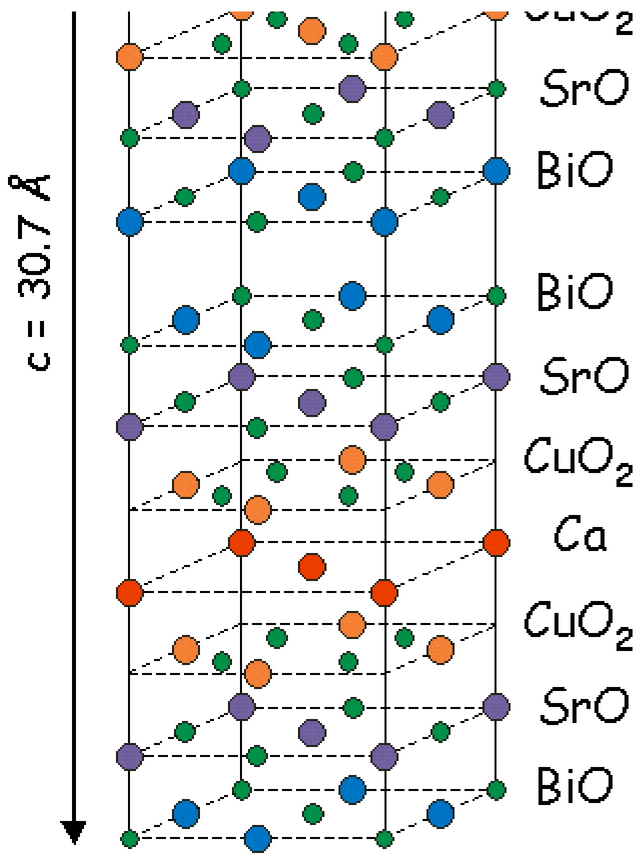
Maksim Velikanov, A.R. and Boris Krippa New J. Phys. 23 033015 (2021)

DMFT: neutron matter at beta-equilibrium



Key questions about High Tc cuprates

$Bi_2Sr_2CaCu_2O_{8+x}$



picture from
http://hoffman.physics.harvard.edu

It is known that the system is correlated

and the coupling is non-local (*d*-pairing)

- What is the pairing mechanism?
- Why Tc is high?
- Why dome structure of the SC state?
- Why planar system?

Going beyond DMFT

Start from the partition function $Z = \int e^{-S[c,c^*]} \mathcal{D}c^* \mathcal{D}c$ with Hubbard action

$$S[c,c^*] = \sum_i S_{imp}[c_i, c_i^*] - \sum_{\omega k \sigma} (\Delta_\omega - \epsilon_k) c^*_{\omega k \sigma} c_{\omega k \sigma}$$

$$S_{imp}[c_i, c_i^*] = \sum_{\omega,\sigma} (\Delta_\omega - \mu - i\omega) c^*_{i,\omega,\sigma} c_{i,\omega,\sigma} + U \int_0^\beta n_{i,\uparrow,\tau} n_{i,\downarrow,\tau} d\tau$$

Use Hubbard-Stratonovich transformation to decouple the *kinetic* part

$$e^{A^2 c^*_{\omega k \sigma} c_{\omega k \sigma}} = B^{-2} \int e^{-AB(c^*_{\omega k \sigma} f_{\omega k \sigma} + f^*_{\omega k \sigma} c_{\omega k \sigma}) - B^2 f^*_{\omega k \sigma} f_{\omega k \sigma}} df^*_{\omega k \sigma} df_{\omega k \sigma}$$

The resulting action

$$S[c, c^*, f, f^*] = \sum_i S_{imp}[c_i, c_i^*] +$$

$$\sum_{\omega k \sigma} \left[g_\omega^{-1} (f^*_{\omega k \sigma} c_{\omega k \sigma} + c^*_{\omega k \sigma} f_{\omega k \sigma}) + g_\omega^{-2} (\Delta_\omega - \epsilon_k)^{-1} f^*_{\omega k \sigma} f_{\omega k \sigma} \right]$$

<u>allows to integrate out *c*, *c** at each site</u>

… yielding

$$S[f,f^*] = \sum_{\omega k\sigma} g_\omega^{-2}\left((\Delta_\omega - \epsilon_k)^{-1} + g_\omega\right) f^*_{\omega k\sigma} f_{\omega k\sigma} + \sum_i V_i$$

$$e^{-V[f_j,f_j^*] - g_\omega^{-1} f^*_{j\omega} f_{j\omega}} = \int e^{-S_{imp}[c_j,c_j^*] + g_\omega^{-1}(f^*_{\omega k\sigma} c_{\omega k\sigma} + c^*_{\omega k\sigma} f_{\omega k\sigma})} \mathcal{D}c_j^* \mathcal{D}c_j$$

$$V[f_i,f_i^*] = -\gamma^{(4)}_{1234} f_1^* f_2 f_3^* f_4 + \gamma^{(6)}_{123456} f_1^* f_2 f_3^* f_4 f_5^* f_6 + \ldots$$

There are exact relations between new and old variables, in particular

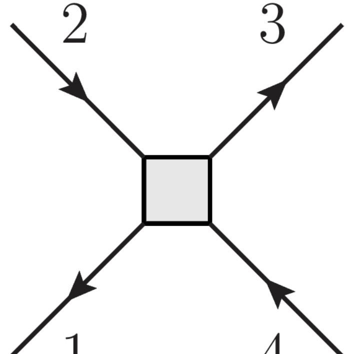
$$G_{\omega,k} = g_\omega^{-2}(\Delta_\omega - \epsilon_k)^{-2} G^{dual}_{\omega,k} + (\Delta_\omega - \epsilon_k)^{-1}$$

Going beyond DMFT: diagrams in dual fermions

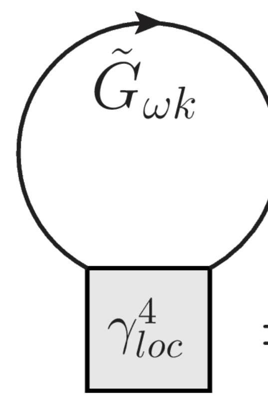
$$S[c,c^\dagger] = \sum_{\omega k \sigma} (-i\omega + \epsilon_k - \mu) c^\dagger_{\omega k \sigma} c_{\omega k \sigma} + U \sum_i \int_0^\beta n_{i\uparrow\tau} n_{i\downarrow\tau}$$

$$S[f,f^\dagger] = \sum_{\omega k \sigma} \underbrace{g_\omega^{-2} \left((\Delta_\omega - \epsilon_k)^{-1} + g_\omega \right)}_{-\tilde{G}_0^{-1}} f^\dagger_{\omega k \sigma} f_{\omega k \sigma} + \sum_n \gamma^{(n)}_{\mathrm{loc}}$$

$$\frac{1}{G_0^{-1}(\omega,k) - \Sigma_\omega} - g_\omega$$

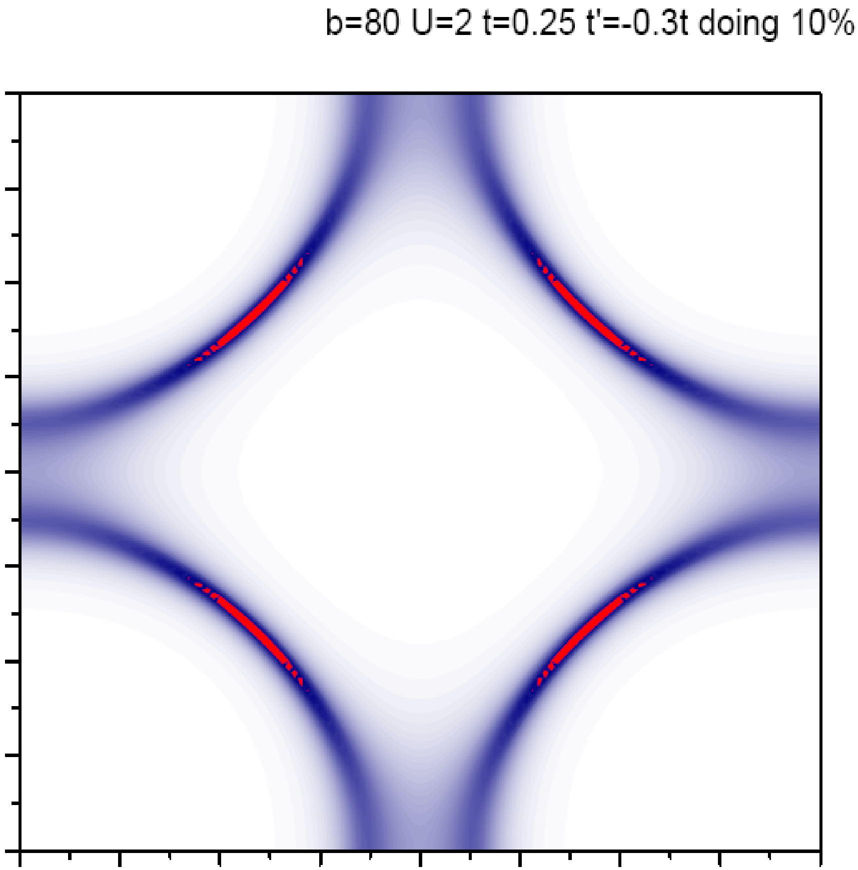


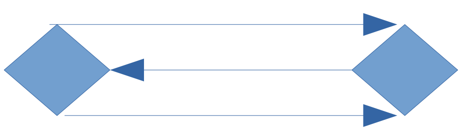
$\gamma^{(4)}_{\mathrm{loc}}$

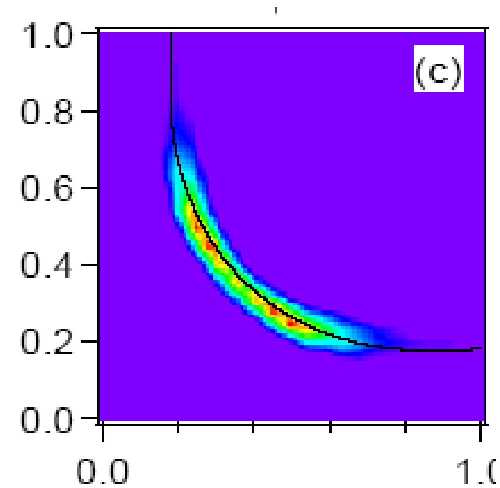


$= 0$

Fermi arcs in cuprates







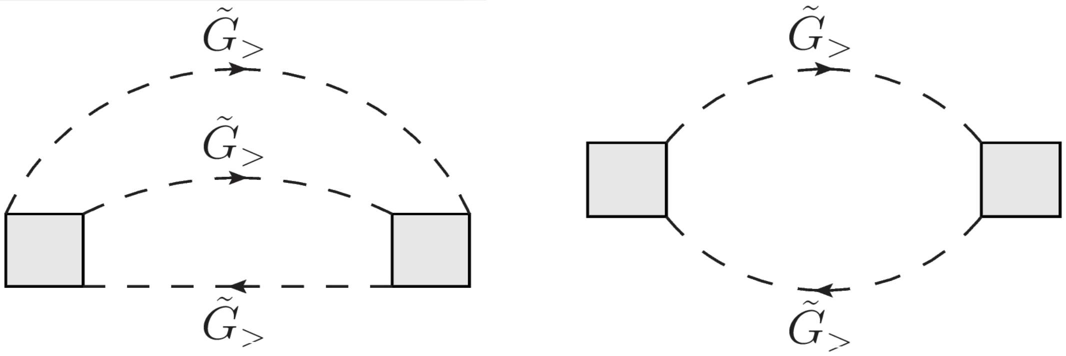
ARPES, Bi2Sr2CaCu208
Norman et al (2007).

ANR, M. I. Katsnelson, A. I. Lichtenstein, A. Georges
Phys.Rev. B 79 045133 (2009)

Low-energy action

$$S[f^\dagger, f] = \sum_{\omega k \sigma} -\tilde{G}_0^{-1} f^\dagger_{\omega k \sigma} f_{\omega k \sigma} + \sum_n \gamma^{(n)}_{\text{loc}}$$

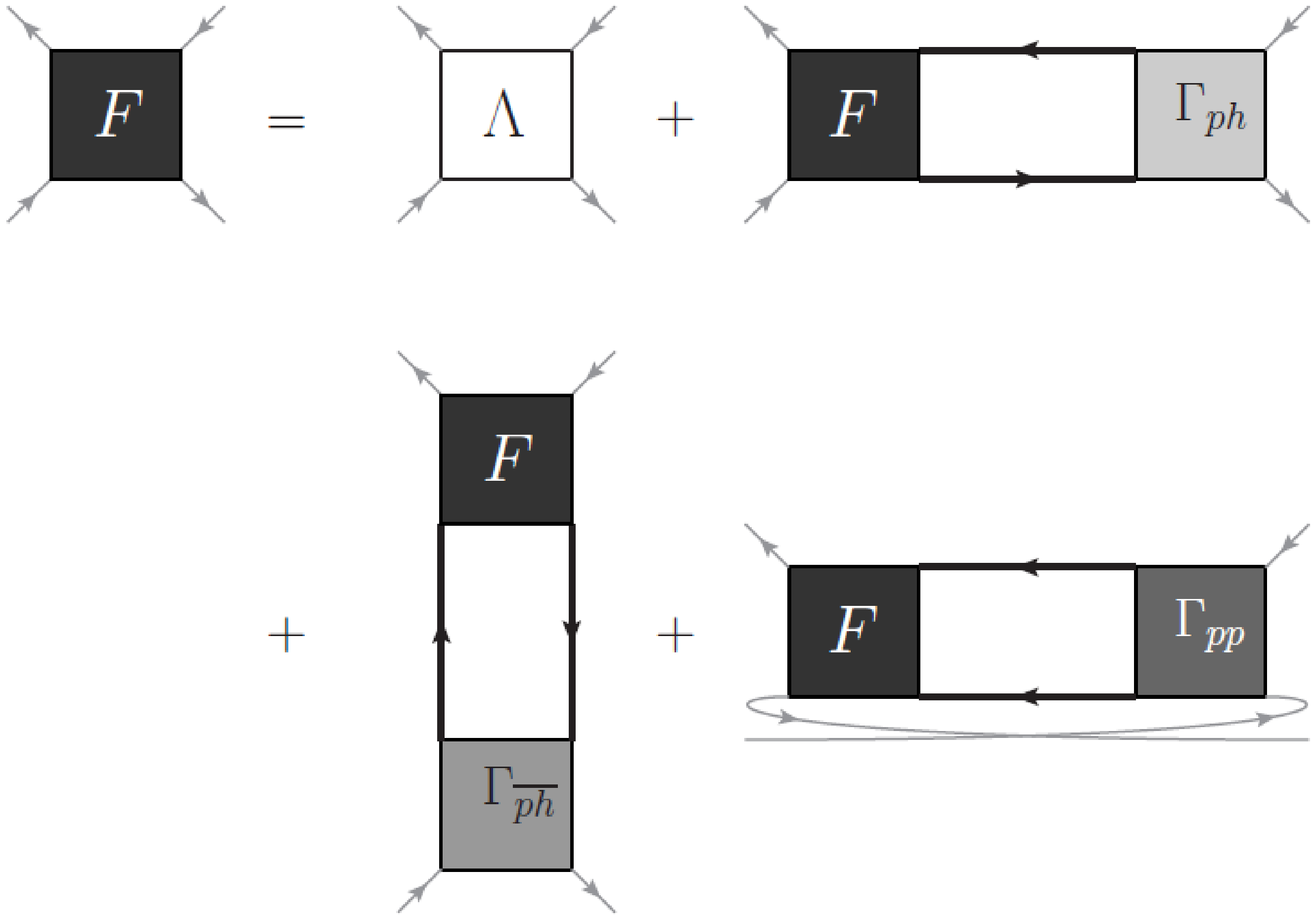
$$S_< = -\sum \mathcal{G}_{12}^{-1} f^\dagger_{1<} f_{2<} + \sum \mathcal{J}_{1234} f^\dagger_{1<} f_{2<} f^\dagger_{3<} f_{4<}$$



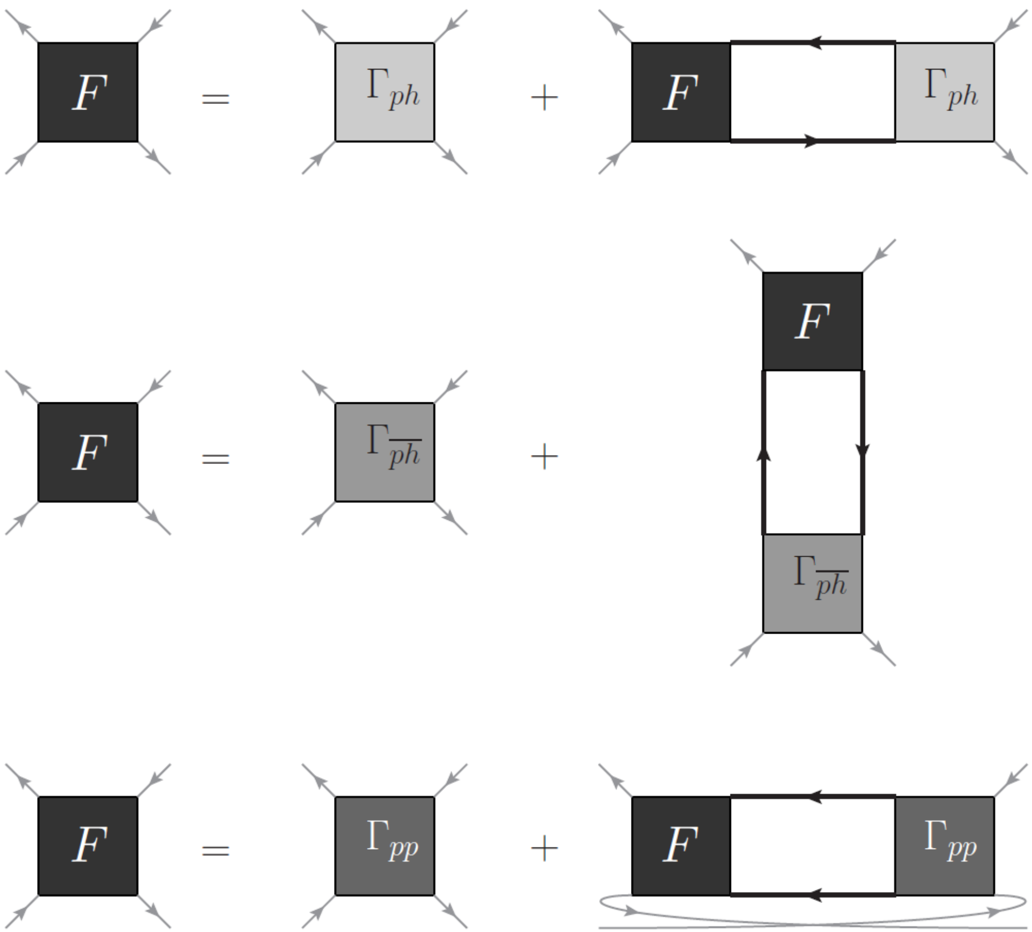
$$f = f_< + f_>$$

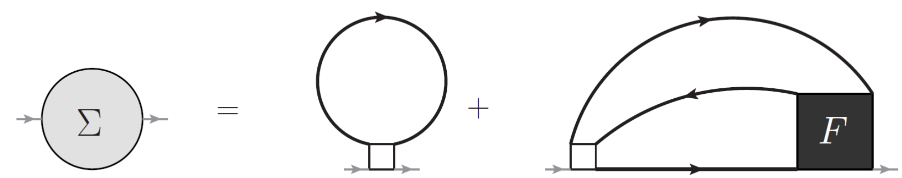
$$f^{(\dagger)}_< = \begin{cases} f^{(\dagger)}_{\omega k \sigma}, & \text{for } |\omega| = \pi T \\ 0, & \text{for } |\omega| > \pi T \end{cases}$$

Parquet formalism: interplay of different channels

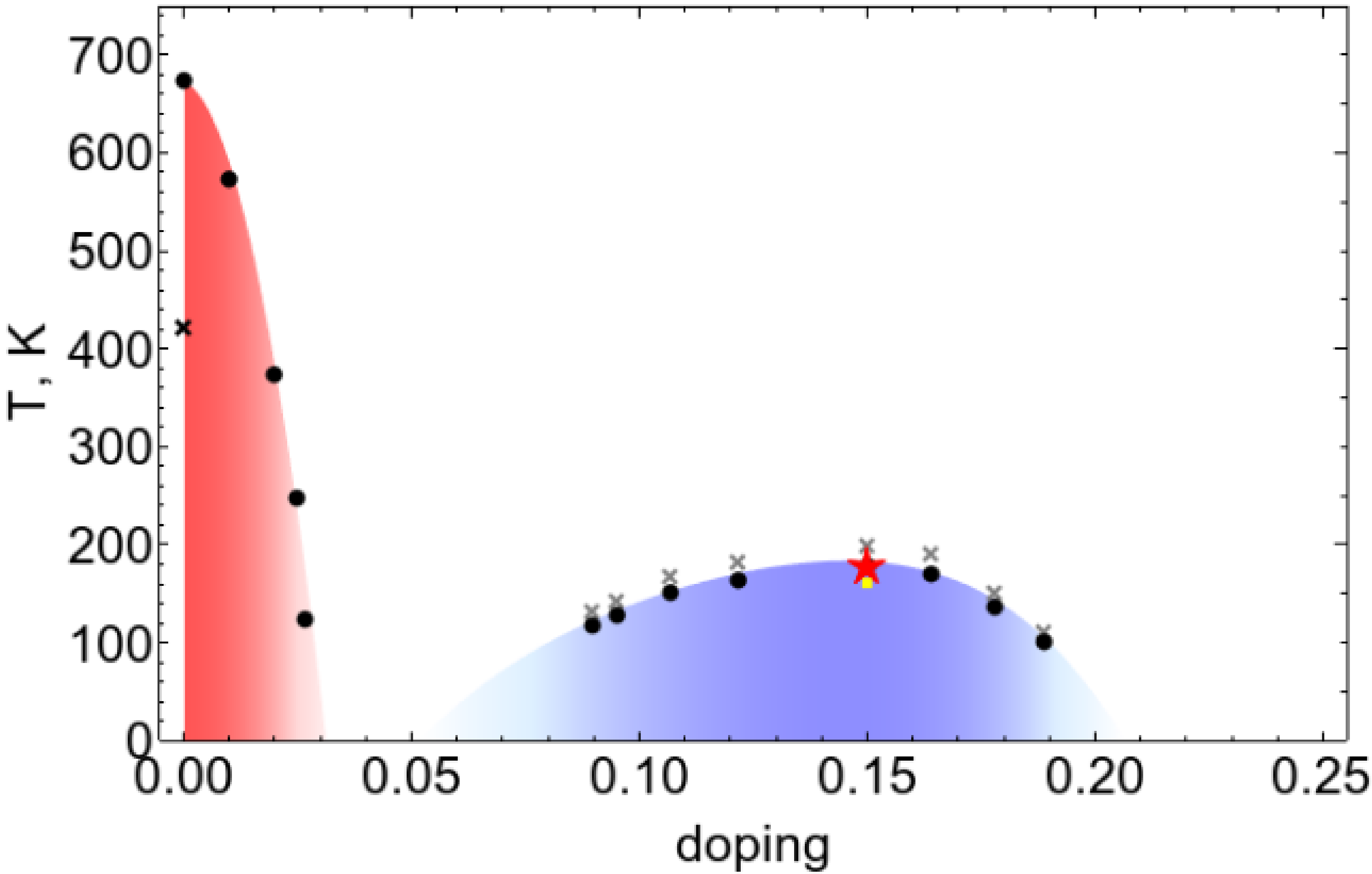


Bethe-Salpeter and Dyson equations



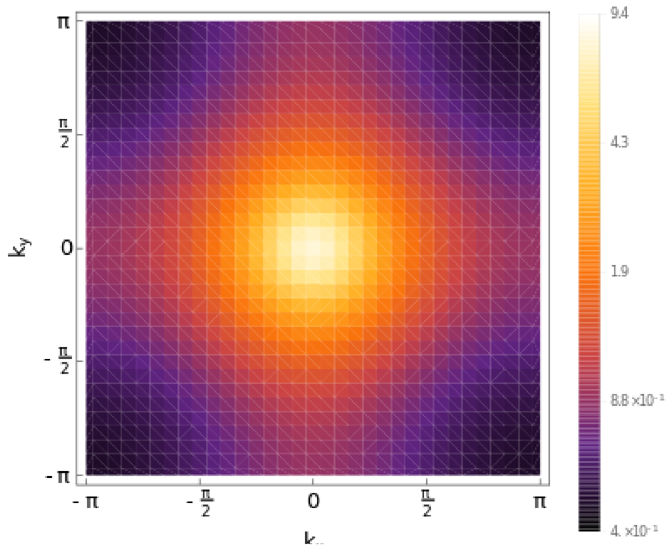


Phase diagram of Hubbard model

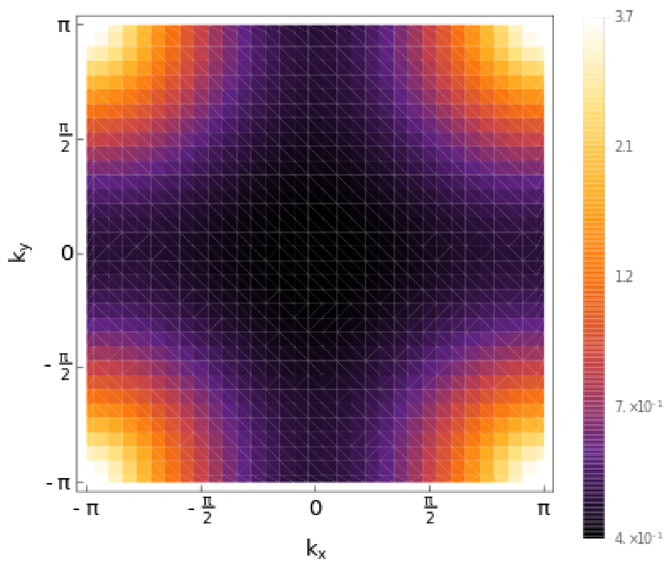


G. V. Astretsov, G. Rohringer, ANR
Phys. Rev. B 101, 075109 (2020)

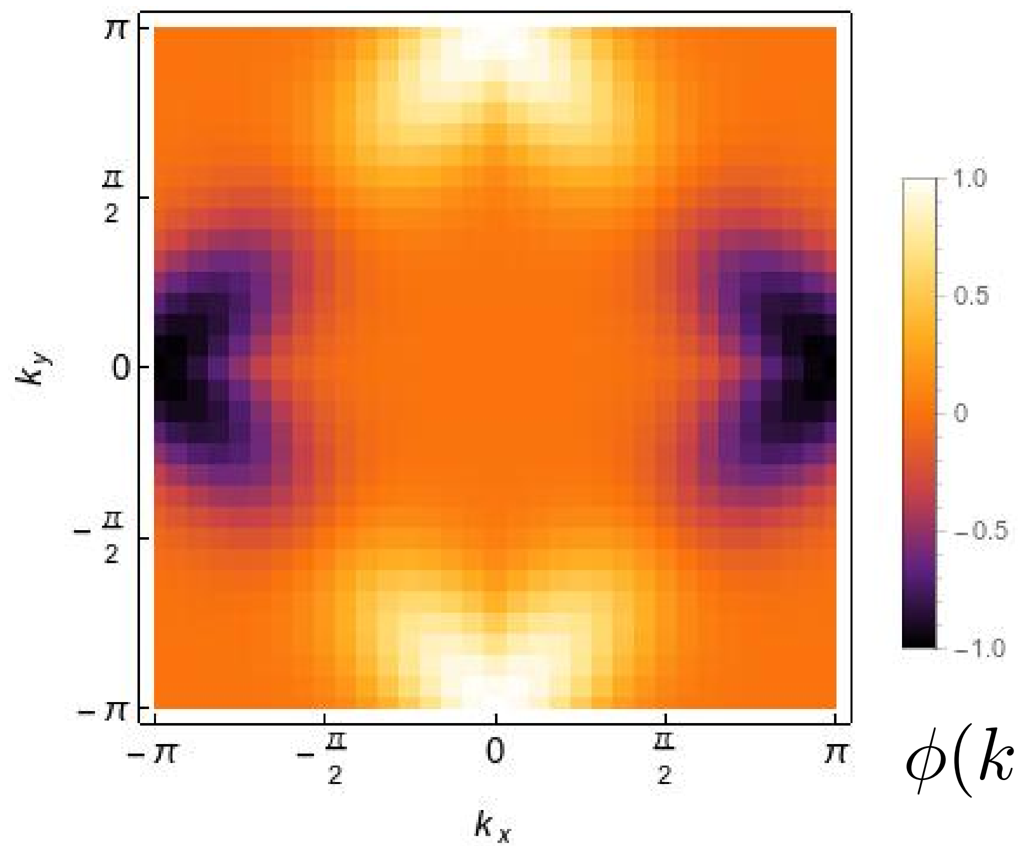
D-wave superconductivity and magnetic fluctuations in Hubbard model



$\chi_{\mathrm{SC}}(k)$



$\chi_{\mathrm{AF}}(k)$



$\phi(k)$

$$(-\chi^0_{\mathrm{pair}}\Gamma^{pp})\phi = \lambda_{SC}\phi$$

- What is the pairing mechanism?

  AF fluctuations

- Why Tc is high?

  Strong coupling of charge carriers with AF modes (no small parameter like m/M)

- Why dome structure of the SC state?

  Interplay of AF fluctuations and DOS of carriers

  van Hove singularities at Fermi level for the optimal doping

- Why planar system?

  2D is a land of fluctuations

  van Hove singularities are stronger in 2D

Hierarchy of scales and approximations

BSCCO

↓

Hubbard

↓

Effective action

↓

L x L

↓

Parquet

- Neglect many-particle local vertices
- Control number of lowest Matsubaras (1, 2…)
- Second order perturbation theory for a renormalized interaction and a propagator

- 16x16 → 32x32 decreases critical temperature

- Self-consistent two-particle method