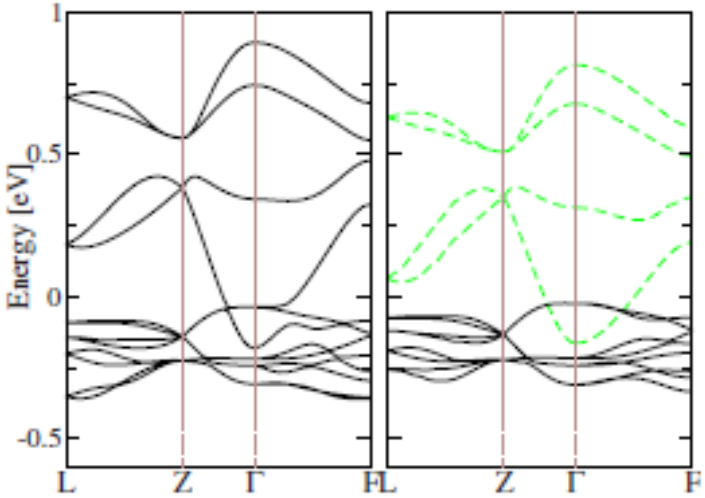
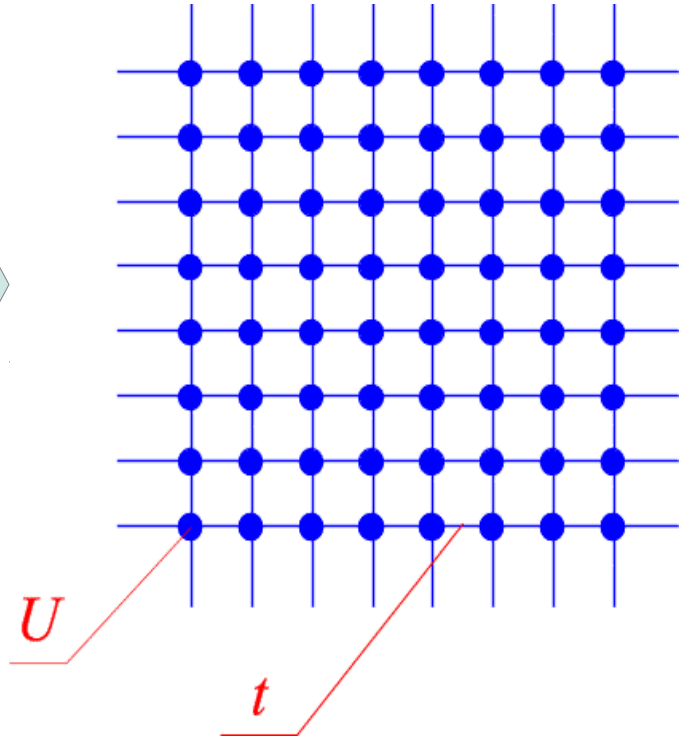
Квантовые методы Монте Карло в теории коррелированных систем

А.Н. Рубцов, МГУ

Сочи 2012

LDA+DMFT framework (beginning)

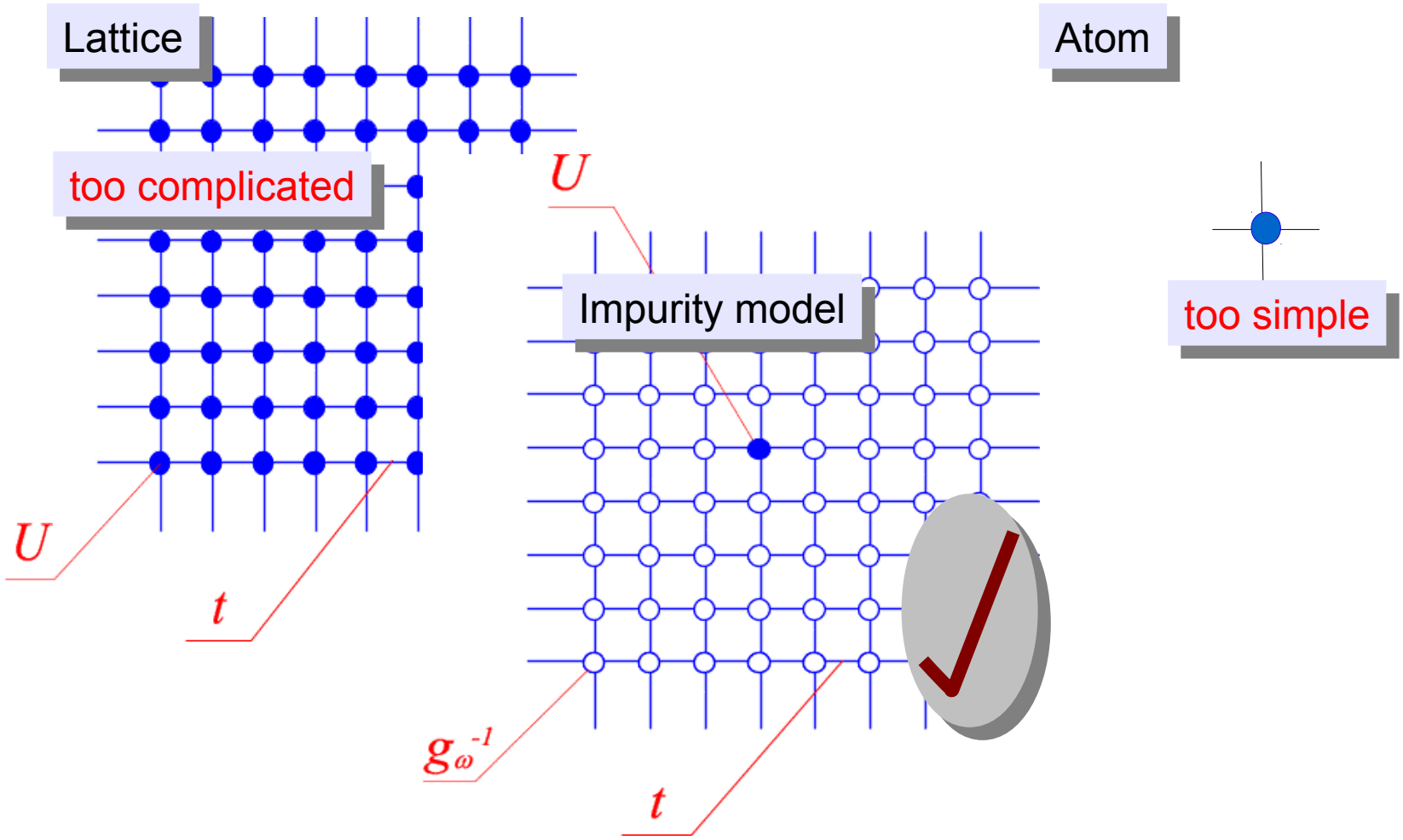




LDA+DMFT V2O3 quasiparticle bands obtained by truncating the self-energies. The left-hand panel gives the eigenvalues of the renormalized Hamiltonian and the right-hand side gives the pure *eg* black and *a*1*g* dashed green band structure (from PhysRevB_76_085127)

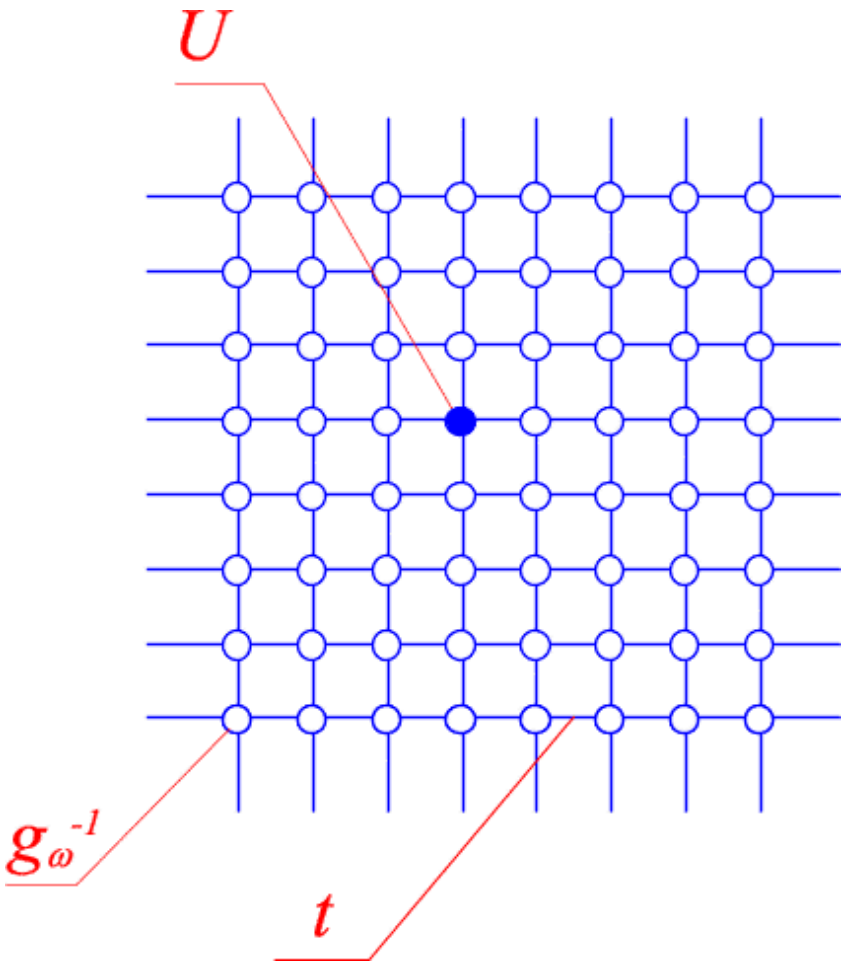
V. Anisimov, et al. J. Phys. CM **9**, 7359 (1997)
A. Lichtenstein, et. al. PRB, **57**, 6884 (1998)

Models systems



DMFT impurity problem

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

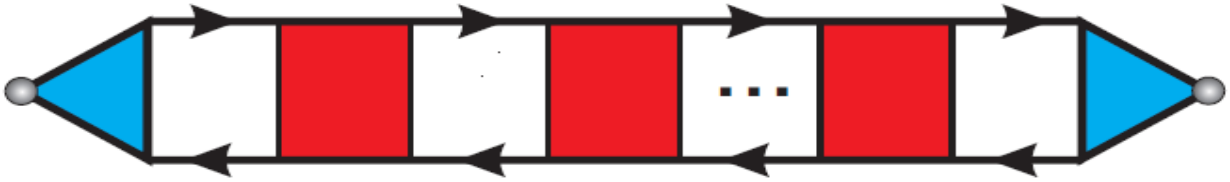


$$g_\omega = \sum_k \frac{N^{-1}}{g_\omega^{-1} - \epsilon_k + \Delta_\omega}$$

$$G_{\omega k} = \frac{1}{g_\omega^{-1} - \epsilon_k + \Delta_\omega}$$

Beyond DMFT

- DMFT is the best local approximation
- Going nonlocal means either cluster flavors of DMFT or expansion around DMFT
- Collective excitations are essentially nonlocal
- Vertex parts (or, equally, many-particle Green's function) of the impurity problem needed



Dual ladder diagram for magnons
Annals of Physics **327** 1320 (2012)

Mathematics behind Monte-Carlo methods

In Monte-Carlo methods, statistical and(or) quantum average is replaced with an average over Markov random walk

$$< G >= \frac{\overline{G_K w_K}}{\overline{w_K}}$$

Here random walk is performed over certain ensemble of auxiliary systems {*K*}; we should be able to calculate G_K and prove the above equality.

For classical Metropolis Monte-Carlo {K} is an ensemble of possible coordinates {x}.

For world-line Monte-Carlo {K} is an ensemble of imaginary-time trajectories {x(τ)}.

For Hirsch-Fye scheme {K} is an ensemble of auxiliary spins

Algorithms can differ in the ensemble {*K*}

and in the Markov matrix.

Optimal sampling

Averages are estimated stochastically

$$< G >= \frac{\sum_K w_K G_K}{\sum_K w_K} = \frac{\overline{w_K G_K p_K^{-1}}}{\overline{w_K p_K^{-1}}}$$

Minimization of the variance

$$\overline{\left(w_K (G_K - < G >) p_K^{-1}\right)^2} = \min, \quad \sum_K p_K = 1$$

Gives

$$p_K \propto |w_K (G_K - < G >)|$$

The most known is so-called importance sampling

$$p_K \propto |w_K|$$

Markov walk

Elementary moves satify

1) Detailed balance

(if one tries to go from *K* to *K'*, he also tries moves from *K'* to *K*)

2) Metropolis acceptance criterion

$$p_{K \to K'} = \min\left(\frac{p'_K}{p_K}, 1\right)$$

Normally, K and K' are ``similar''.

+ easy calculation of $p_{K \to K'}$
+ good acceptance rate
- autocorrelations

$$\delta G \approx \sqrt{\frac{D^2(G) N_{autocorr}}{N}}$$

Fermionic algorithms prior to CT-QMC

Hubbard-Stratonovich transformation:

R. L. Stratonovich, 1957

J. Hubbard, 1959

D. J. Scalapino and R. L. Sugar, 1981

Discrete transformation:

J.E. Hirsch (Phys. Rev. B 28, p.4059, 1983)

$$e^{-\delta\tau U\hat{n}_\uparrow\hat{n}_\downarrow+\hat{A}} \approx \frac{1}{2}\sum_{s=\pm1} e^{s\sqrt{\delta\tau U}(\hat{n}_\uparrow-\hat{n}_\downarrow)-\delta\tau U(\hat{n}_\uparrow+\hat{n}_\downarrow)+\hat{A}}$$

No time discretisation:

S.M.A.Rombouts, K.Heyde, and N.Jachowicz (1999)

Interaction expansion

can be any $(G^{(0)})^{-1}$

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

W

Consider the series with respect to *W* (in the interaction representation)

$$Z = \mathrm{Sp} T e^{-\int W^0(\tau) d\tau}, \quad G(\tau,\tau') = Z^{-1}\mathrm{Sp} T c^{\dagger}(\tau) c(\tau') e^{-\int W^0(\tau) d\tau}$$

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

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

Idea of algorithm is

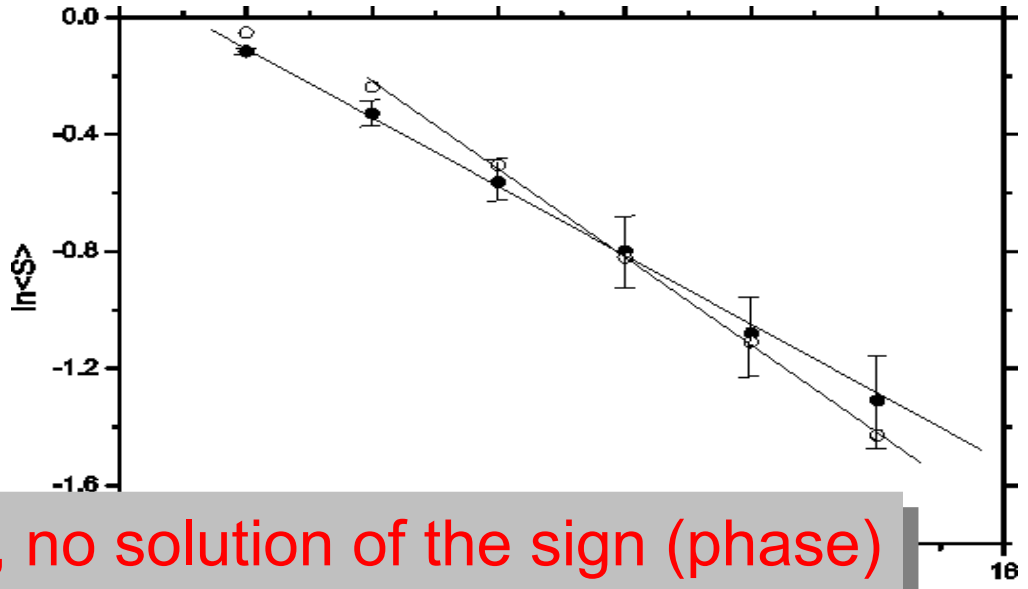
to perform a random walk in the space of {k, (arguments of integrals)} .

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

Optimizing the average sign

"Trivial" sign problem:

Idea of solution:



Interact

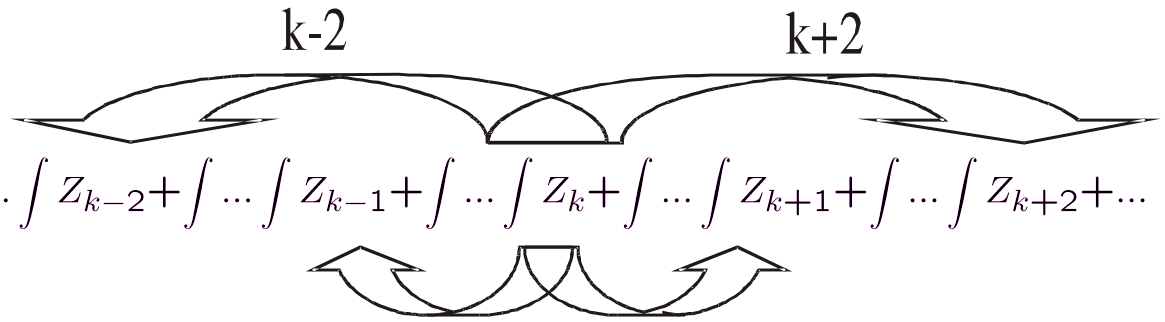
For real-time evolution, no solution of the sign (phase) problem is known

.05.

Random walk in K-space

Call state K the set

$$K = k, t_1 ... t_k, r_1 ... r_k$$



and perform a random walk with probability density

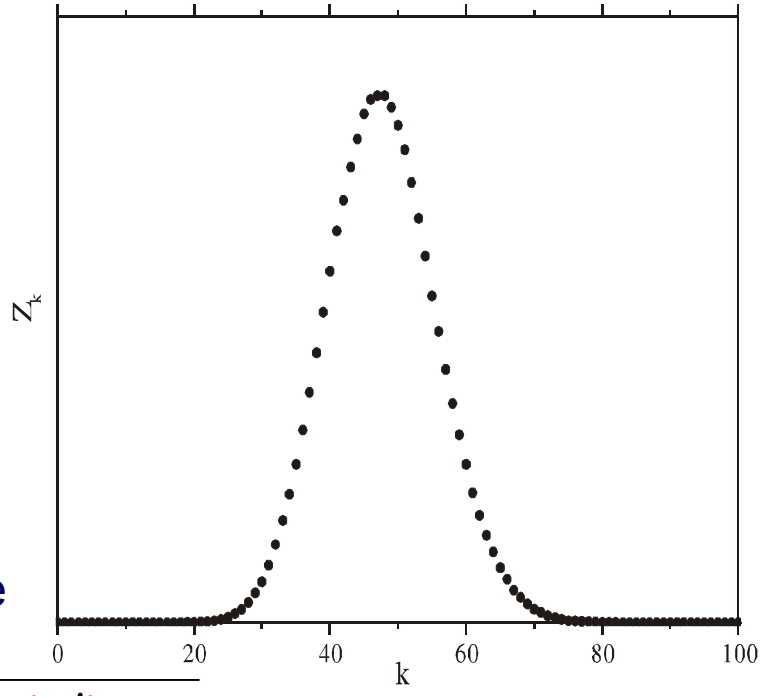
$$p(K) \propto Z_k = \mathrm{Sp} T W_0(\tau_1, r_1) ... W_0(\tau_k, r_k)$$

Trace here can be explicitly calculated from the Wick theorem (H_0 is Gaussian!)

$$< T c_1^\dagger c_1 ... c_k^\dagger c_k = \det ||g_{ij}||$$

It is possible to prove that for such an ensemble

$$G = \overline{g_0}, \text{ or } < T c^\dagger(\tau) c(\tau') > = \overline{< T c^\dagger(\tau) c(\tau') >_0}$$



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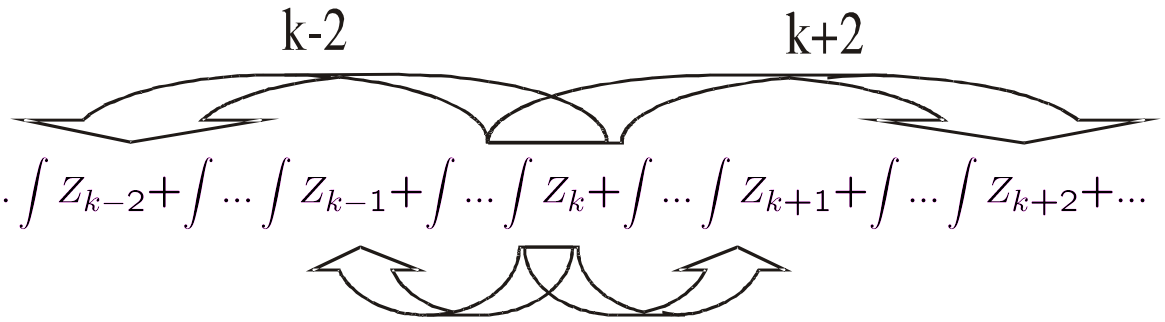

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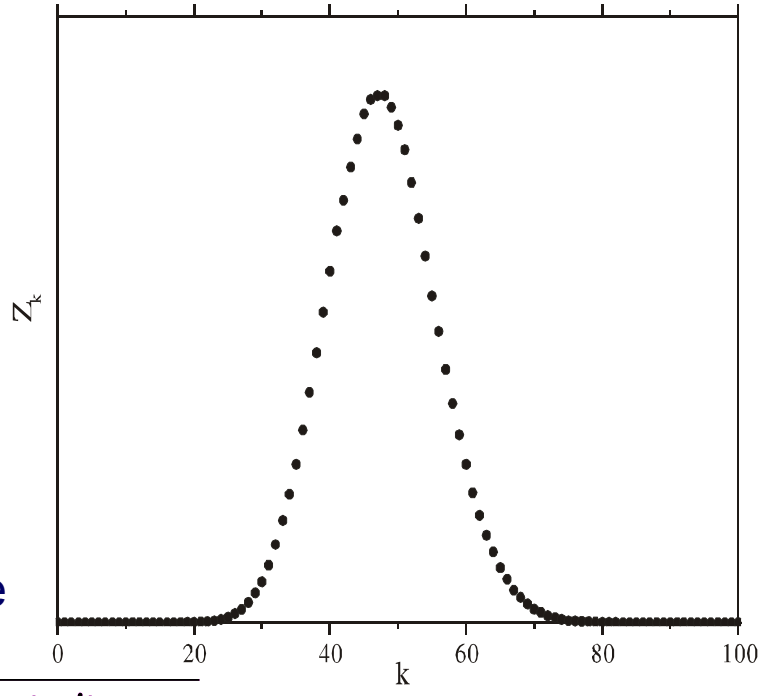
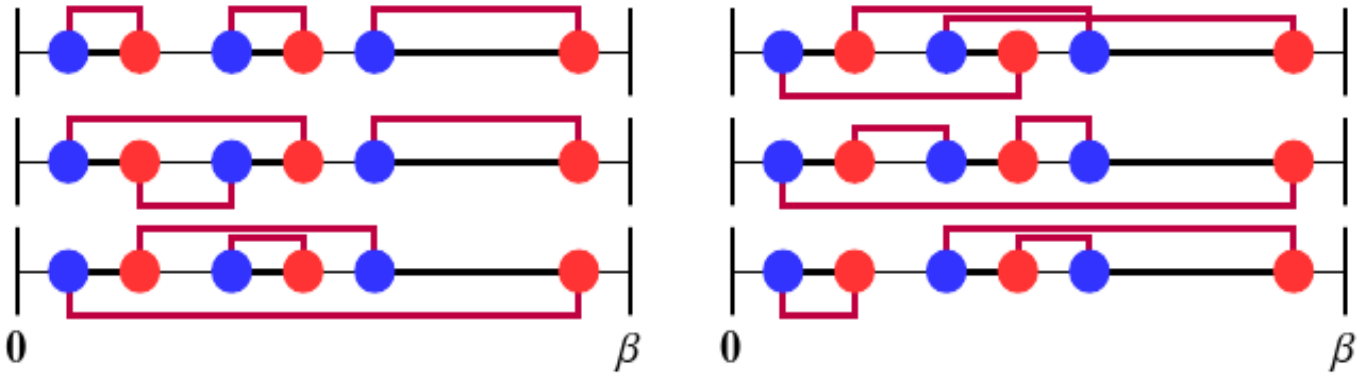


Strong-coupling expansion

$$S = S_{at} + \Delta_{\tau-\tau' s s'} c^{\dagger}_{s\tau} c_{s'\tau'}$$

The idea is to expand in hybridization

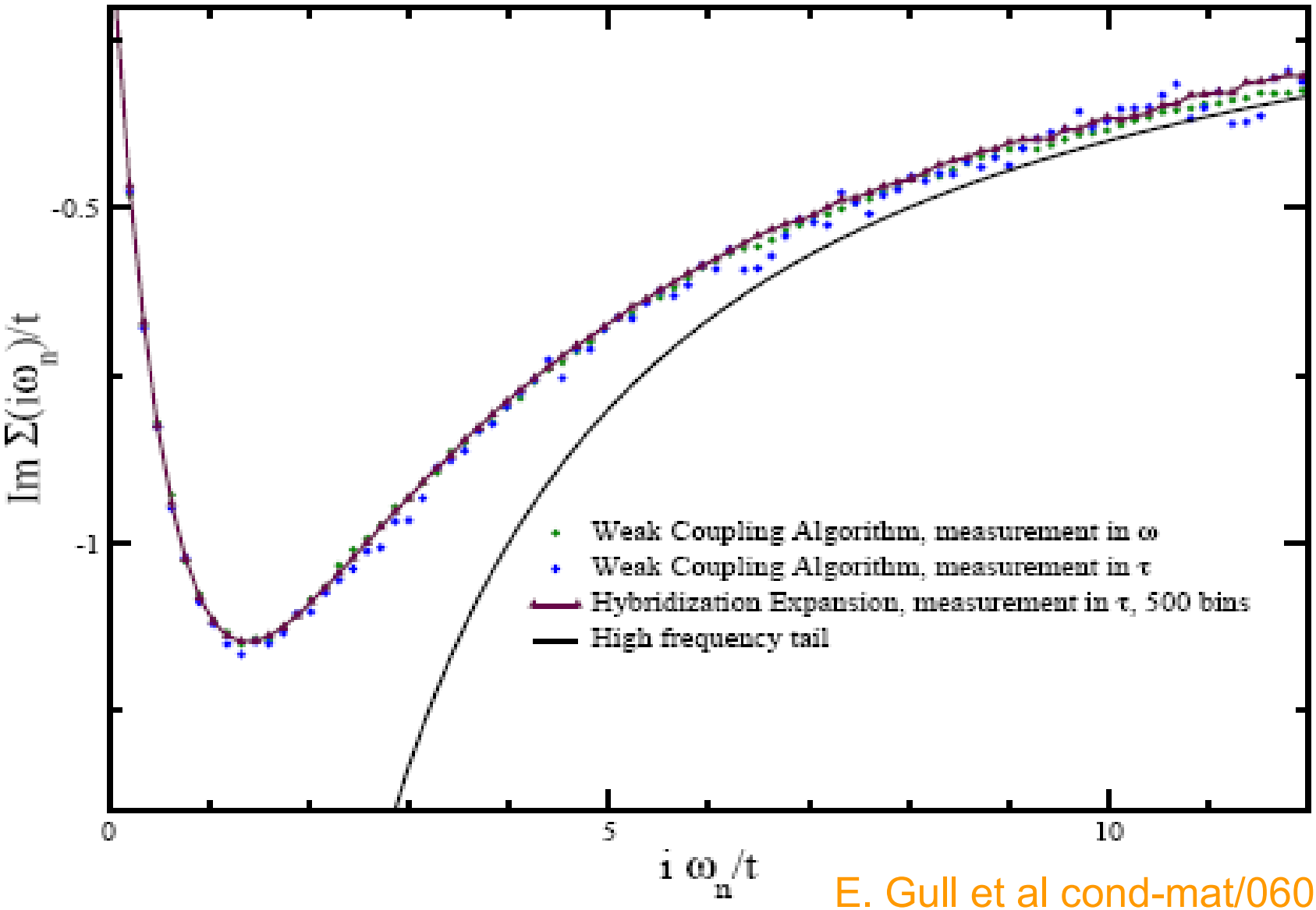


"Метод интегрирования по траекториям ... фактически никогда не был полезен при рассмотрении вырожденных Ферми-систем"

Р. Фейнман, А.Хиббс

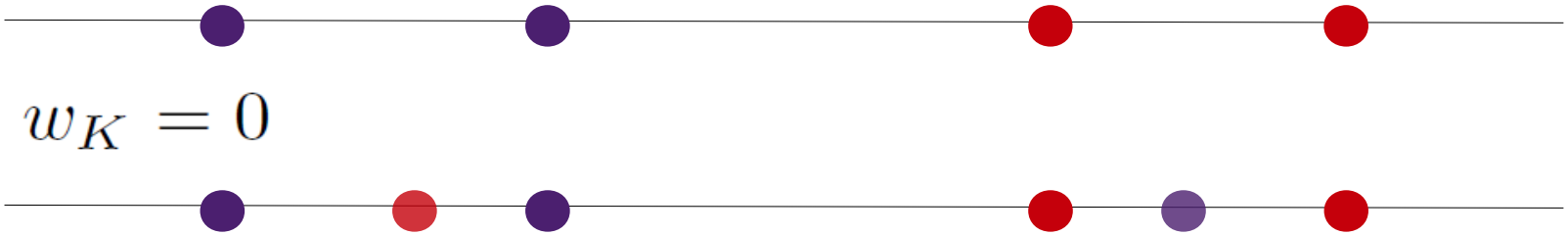
Квантовая механика и интегралы по траекториям

Calculation with different CT-QMC schemes



E. Gull et al cond-mat/0609438

Optimum sampling



$w_K = 0$

$w_K G_K \neq 0$

Recall

$$< G >= \frac{\sum_K w_K G_K}{\sum_K w_K} = \frac{\overline{w_K G_K p_K^{-1}}}{\overline{w_K p_K^{-1}}}$$

Importance sampling

$$p_K \propto |w_k(G_K - < G >)| \approx |w_k|$$

Better take

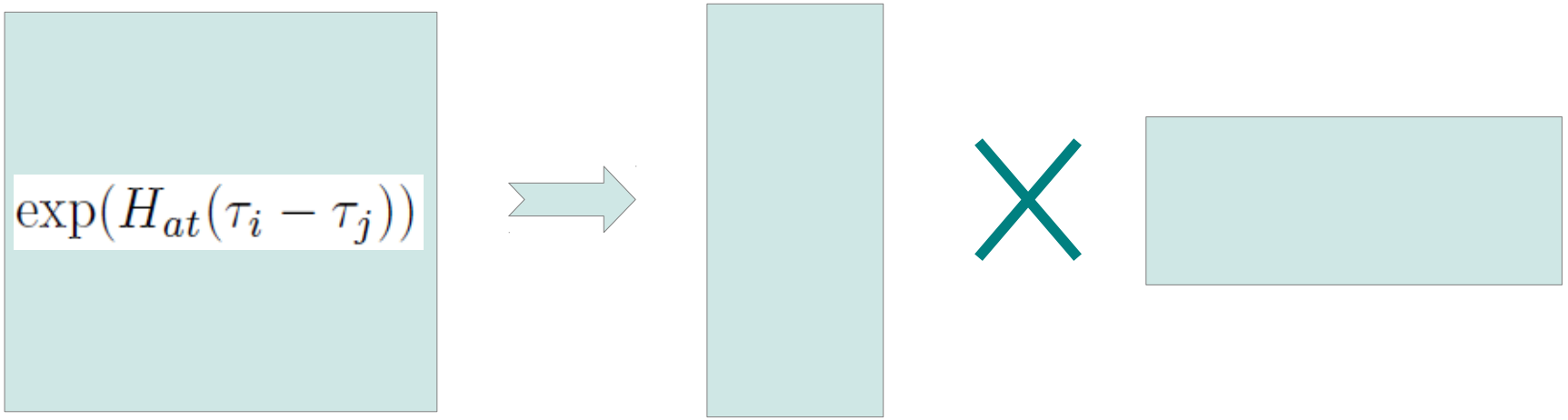
$$p_K \propto |w_k(G_K - < G >)| \approx |w_k| \sqrt{G_K^2 + 1}$$

Speeding up:

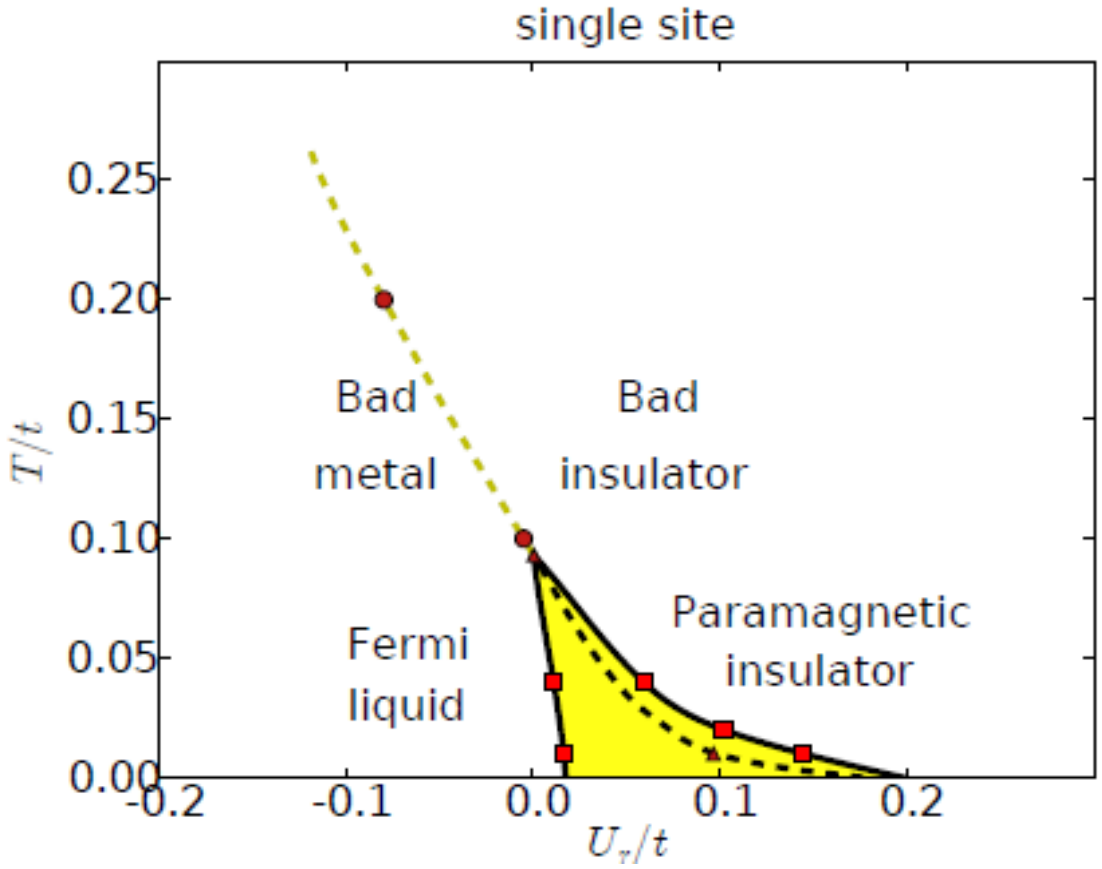
Fast updates

$$(A + x \cdot y)^{-1} = A^{-1} - \frac{A^{-1}x \cdot yA^{-1}}{1 + (yA^{-1}x)}$$

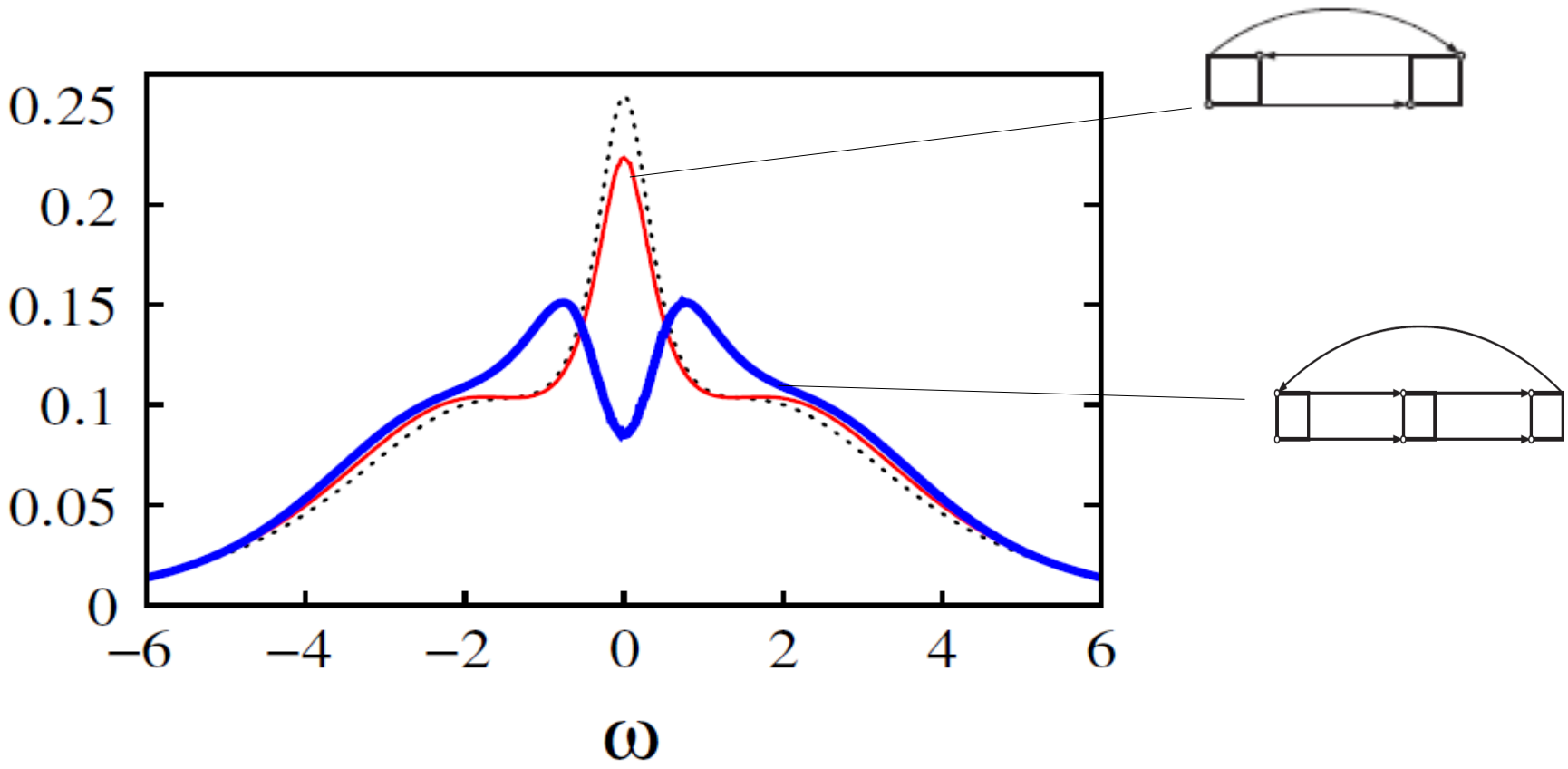
Krylov method



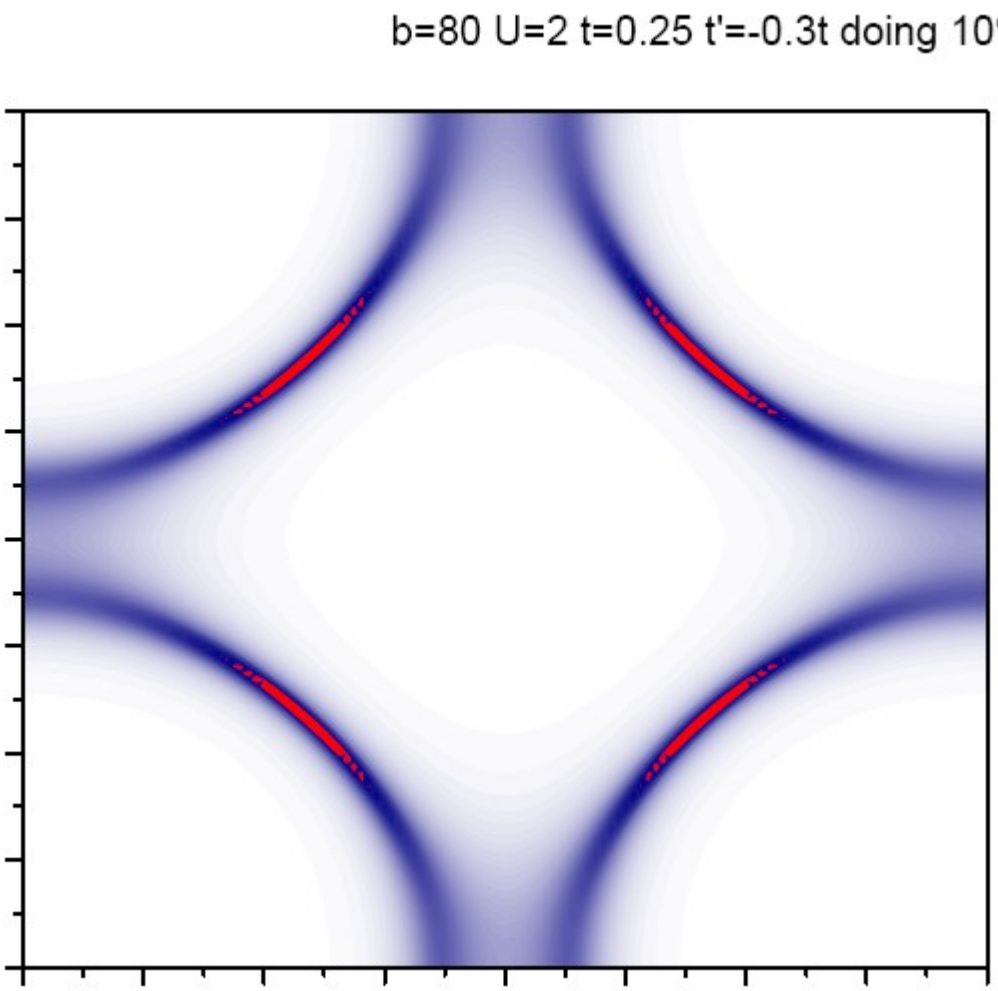
DMFT phase diagram of Hubbard model

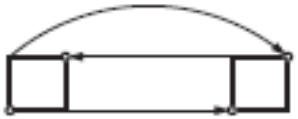


DF calculation of ``paramagnetic'' pseudogap in Hubbard model

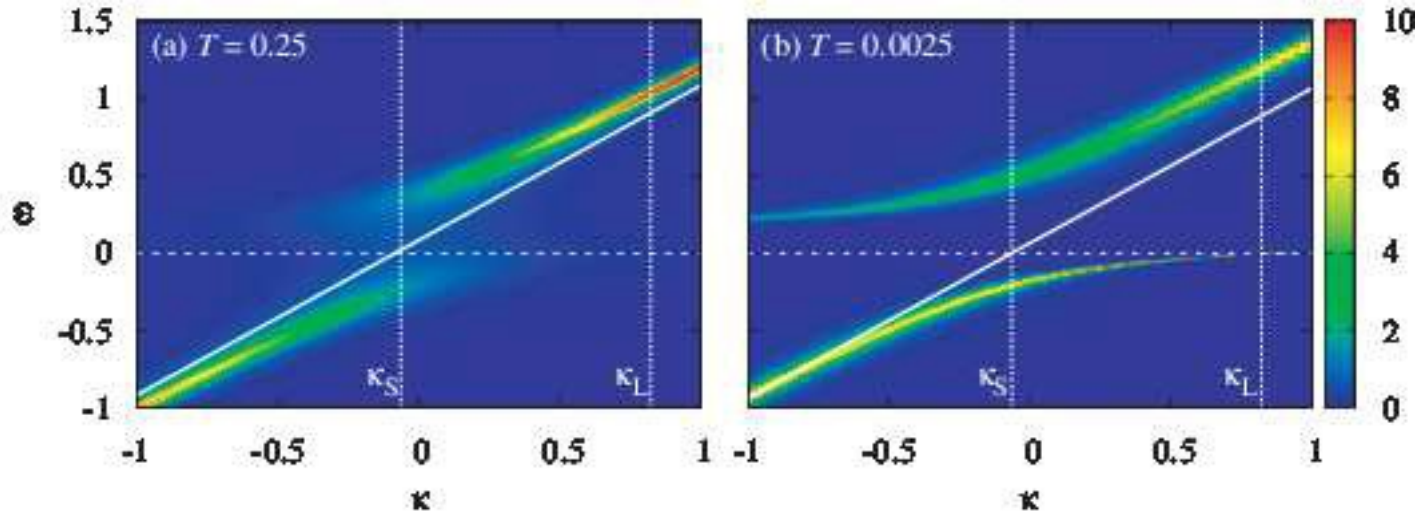


DF calculation of Fermi arcs in doped Hubbard model





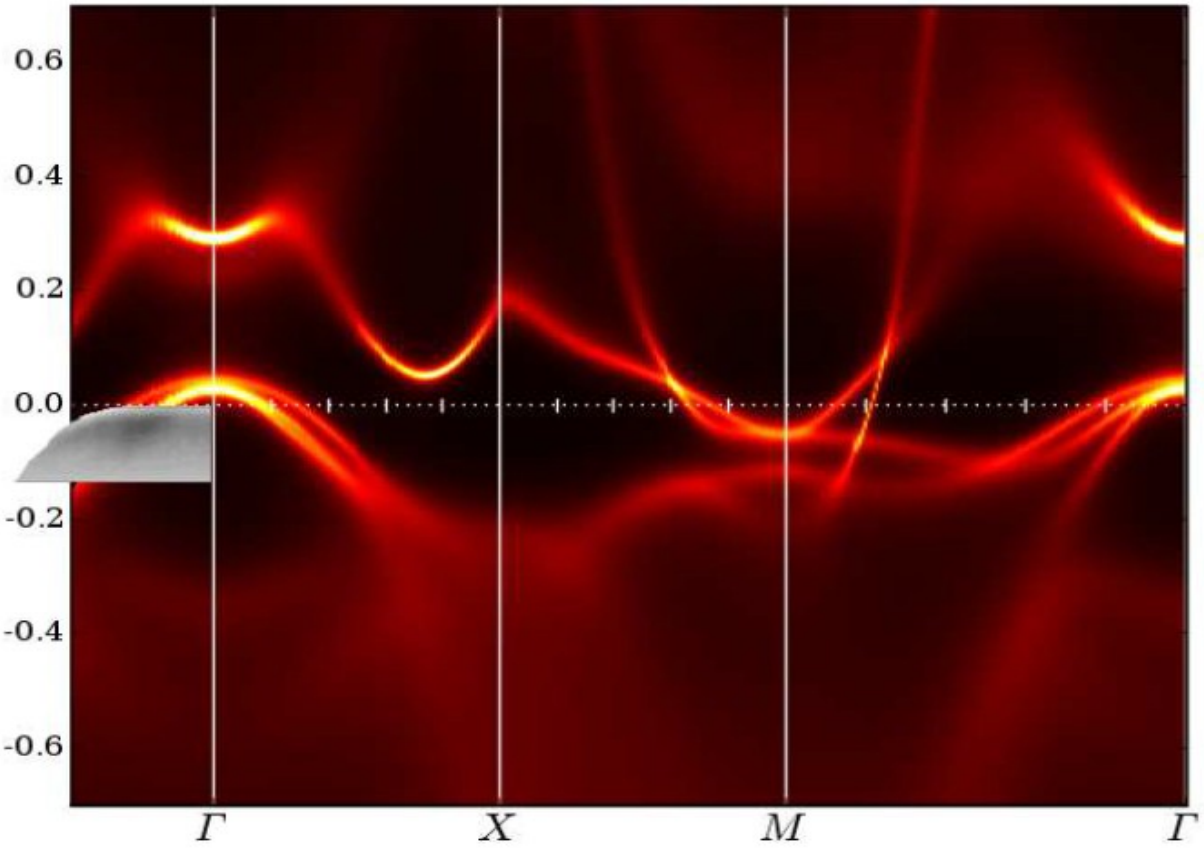
Studies of a Kondo lattice model



The single-particle excitation spectrum for J = 0.3 and nc = 0.9 at (a) T = 0.25 and (b) T = 0.0025

Otsuki, J., H. Kusunose, and Y. Kuramoto (2009), Phys. Rev. Lett. 102 (1), 017202

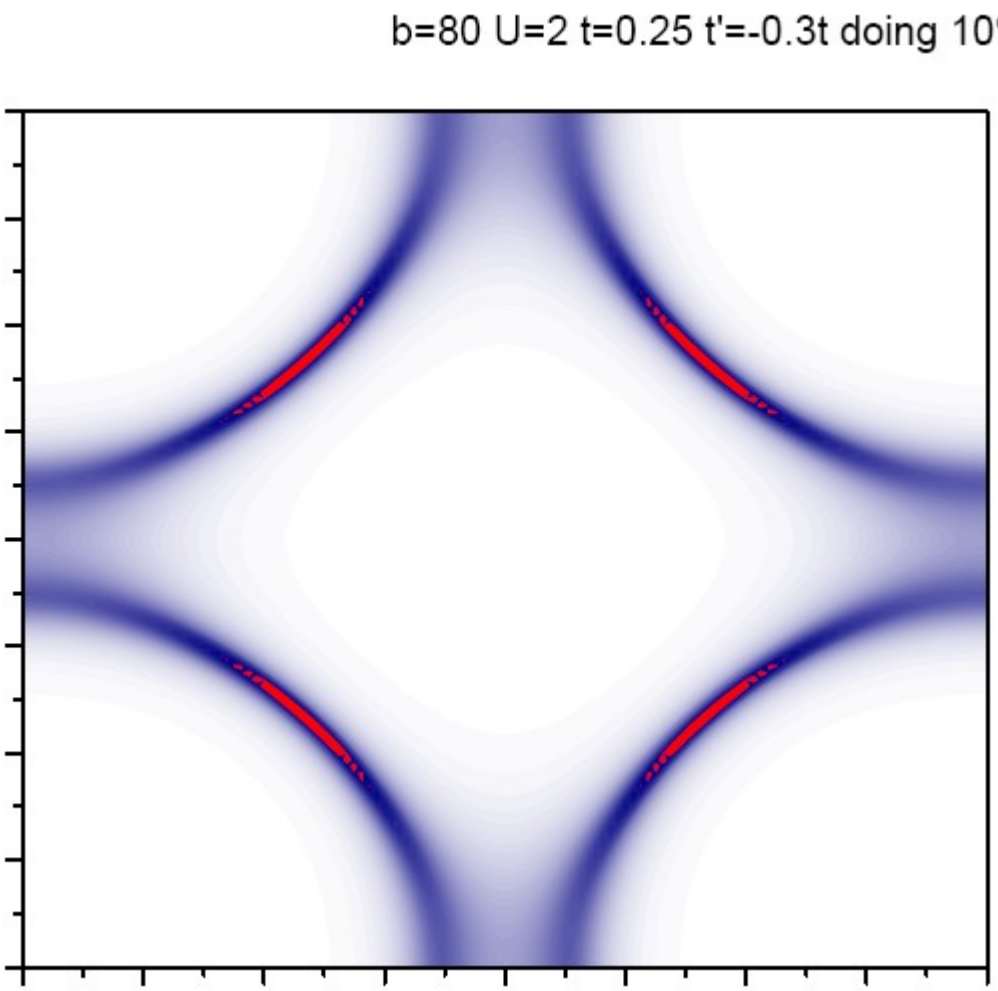
Real materials, multiorbital models

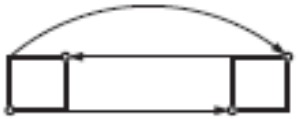


Momentum resolved spectral function calculated for BaFe2As2

Kutepov, A., K. Haule, S. Y. Savrasov, and G. Kotliar (2010), Phys. Rev. B 82 (4), 045105

DF calculation of Fermi arcs in doped Hubbard model





Main problems at the moment:

- more effective multiorbital algorithms
- real-time CT-QMC

For a review:

E. Gull, A.J. Millis, A.I. Lichtensten, A.N. Rubtsov, M.Troyer, Ph. Werner
Continuous-time Monte Carlo methods for quantum impurity models
Reviews Of Modern Physics – 2011 – V.83 P.349