Extremely Correlated Quantum Liquids

ECQL

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Work supported by
NSF DMR 0706128

Work supported by
DOE, BES DE-FG02-06ER46319

General Motivation

Search for Non Fermi liquids

Strong interactions in doped Mott insulators

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

Hubbard model (t,U)

J= 4 t^2/U

t J Model

t,J
independent

Multi band models

$$H = -\sum_{i,j} t_{i,j} \; P_G \; c^\dagger_{i,\sigma} c_{j,\sigma} \; P_G + J \sum_{\langle i,j \rangle} \; \vec{S}_i \cdot \vec{S}_j$$

P_G=Gutzwiller Projector

Passage from Strong Correlations to Extreme Correlations

$$U \gg zt \qquad\qquad U = \infty$$

Use "Schwinger's way" + asymptotic freedom of vertex

Leo Tolstoy: (Anna Karenina)

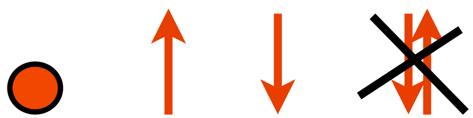
All Fermi liquids are all alike;

Each Non Fermi liquid is Non Fermi in its own way.

$$P_G = \prod_j (1 - n_{j\uparrow} n_{j\downarrow})$$ Gutzwiller projector

$1 \leq j \leq N_s$ $\quad N_s =$ number of sites

$X_j^{\sigma 0} = P_G \; c_{j\sigma}^{\dagger} \; P_G$ $\quad X_j^{0\sigma} = P_G \; c_{j\sigma} \; P_G$ Non canonical Fermi operators



Three allowed configurations after Gutzwiller projector

$$U \longrightarrow \infty$$

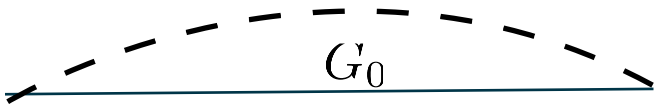
Hilbert space has fewer states after projection:

3^{N_s} rather than 4^{N_s}

- A classic example of singular perturbation: Discussed in QM by John Klauder as "Footprints of the dinosaurs"
- Changes the rules of quantum mechanics: Non canonical objects (X's) and smaller dimension of Hilbert space.
- Lattice is crucial- in the continuum, a strong coupling is usually more benign- "Bruckner-izable"
- When $N_e = N_s$, get an insulating state where electrons are stuck at their home base- Mott Insulator with no analog in the continuum.

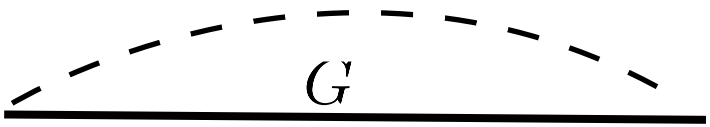
The "Feynman way"

Self energy in terms of G_0 using Wicks theorem and Feynman diagrams



And then "discover"

Skeleton Graph expansion, i.e. omit s.e. insertions in intermediate diagrams and replace G_0 by G
Generates Self energy in terms of G



The "Schwinger way"

Schwinger directly generates self energy in terms of full G
Does not need or use Wick's theorem!!

Unlike BBGKY hierarchy, Schwinger Dyson works with inverse of Greens function, hence much more powerful

Dyson Schwinger expansion is analogous to Stieltjes expansion of power series in continued fractions

$$\frac{b_0}{z} + \frac{b_1}{z^2} + \frac{b_2}{z^3} + \ldots = \cfrac{a_0}{z + \cfrac{a_1}{z + \cfrac{a_2}{z + ..}}}$$

$\sim \Sigma(z)$


Scanned at the American
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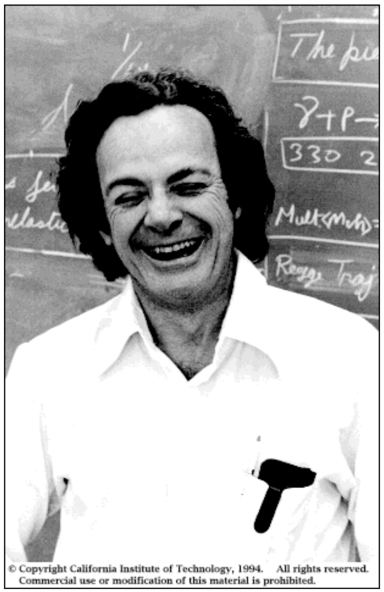
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Paul Martin quote:
(Climbing the Mountain: Biography of Schwinger)

…"In the dark recesses of the sub-basement of Lyman Laboratory, where theoreticians retired to decipher their tablets, and where the ritual taboo on pagan pictures could be safely ignored, students scribbled drawings that disclosed profound identities between diagrams and sums of diagrams."

"As to the conversations we held with him as graduate students, he might frown when one of us drew a Feynman diagram, but we knew all about those diagrams, including how to generate them quickly and concisely from functional equations **that bypassed Wick theorems*** and the like."

(*emphasis added)

The Problem:

- ★ Non Canonical Field Theory: Challenging Frontier
- ★ How to handle Gutzwiller projection within field theory rigorously.
- ★ A central problem in Condensed Matter Physics: From Strong correlations to Extreme Correlations.

The proposed Solution:

•**Step1**: Use Schwinger's source idea to generate exact Equation of Motion for Greens function.
•**Step 2**: Require ***Asymptotic Freedom of Vertex Functions*** at high energy- achieved through a factorization

PHYSICAL REVIEW B **81**, 045121 (2010)

Extremely correlated quantum liquids

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Rather long paper: 30 pages
Details of calculations 8 appendices:
A new formalism that parallels the Fermi Liquid treatment using vertex functions a la Martin + Schwinger+Kadanoff+Baym+ Rajagopal

- Highlights of paper:
- Non Perturbative treatment of tJ model: Exact formulation
- Key results including exact expression for self energy in the tJ model in terms of vertex
- Schwinger Dyson Hierarchy of equations for vertices

Start with deriving the exact Equation of Motion for tJ model:

$$X_i^{\sigma_1\sigma_2} = |\sigma_1\rangle\langle\sigma_2|, \quad \underbrace{X_i^{0\sigma_1} = |0\rangle\langle\sigma_1|}_{\sim c}, \quad X_i^{\sigma_1 0} = |\sigma_1\rangle\langle 0|, \quad \sim c^\dagger$$

$$X_i^{ab} X_i^{cd} = \delta_{bc} X_i^{ad}$$

$$\{X_i^{0\sigma_1}, X_j^{\sigma_2 0}\} = \delta_{ij}[\delta_{\sigma_1\sigma_2} - \sigma_1\sigma_2 X_i^{\bar{\sigma}_1\bar{\sigma}_2}].$$

Hubbard X operators are non canonical:
Their (graded) Lie algebra is a variation of the Fermionic one.
Projecting out double occupancy changes the algebra.

$$\mathcal{G}_{\sigma_1\sigma_2}[1,2] = -\frac{Tr\left[e^{-\beta H} T(e^{-\mathcal{A}}\ X_1^{0\sigma_1}(\tau_1) X_2^{\sigma_2 0}(\tau_2))\right]}{Tr\left[e^{-\beta H} T(e^{-\mathcal{A}})\right]}$$

$$\boxed{\mathcal{G}_{\sigma_i\sigma_f}[i,f] = -\langle\langle X_i^{0\sigma_i}\ X_f^{\sigma_f 0}\rangle\rangle}$$

i,f gives space-time points

$$\mathcal{A} = \sum_{j,\sigma_1,\sigma_2} \int_0^\beta d\tau\ \mathcal{V}_j^{\sigma_1\sigma_2}(\tau) X_j^{\sigma_1\sigma_2}(\tau)$$

Source term of Schwinger used for generating EOM

The Greens fn is a 2x2 matrix in spin space

$$\Delta[i] = \delta_{\sigma_1,\sigma_2} - \sigma_1\sigma_2\mathcal{G}_{\bar\sigma_2\bar\sigma_1}[i^-, i]$$
$$\rightarrow (1-\frac{n}{2})$$

This (matrix) object Δ[i] plays an important role:
It multiplies the most singular term in the exact EOM

Step 1: Exact EOM

$$\boxed{(\partial_{\tau_i}-\mu)\mathcal{G}[i,f] = -\delta[i,f]\Delta[i] - \mathcal{V}_i\cdot\mathcal{G}[i,f] - X[i,j]\cdot\mathcal{G}[j,f] - Y[i,j]\cdot\mathcal{G}[j,f]}$$

$$X[i,j] = -t[i,j]\ D[i] + \frac{1}{2}J[i,k]\ D[k]\delta[i,j]$$
$$Y[i,j] = -t[i,j]\ \Delta[i] + \frac{1}{2}J[i,k]\ \Delta[k]\delta[i,j]$$

$$D_{\sigma_1,\sigma_2}[r] = \sigma_1\sigma_2\frac{\delta}{\delta\mathcal{V}_r^{\bar\sigma_1\bar\sigma_2}}$$

Non canonical ⇒ the coefficient of δ[i,f] is time dependent: it creates all complications

Step 2: Asymptotic Freedom through Exact Factorization

$$\mathcal{G}[i,f] = \Delta[i] \cdot \hat{G}[i,f]$$

$$(\Delta[i])^{-1} \cdot \partial_\tau \mathcal{G}[i,f] = (\Delta[i])^{-1} \cdot \partial_\tau \Delta[i] \quad \cdot \hat{G}[i,f] + \partial_\tau \hat{G}[i,f]$$

Exact Transformation into Canonical EOM's

$$(\partial_{\tau_i} - \mu + V_i + \Phi_i)\hat{G}[i,f] = -\delta[i,f] - (\Delta^{-1}[i] \cdot X[i,j] \cdot \Delta[j] + \Delta^{-1}[i] \cdot Y[i,j] \cdot \Delta[j]) \cdot \hat{G}[j,f]$$

Can solve for Δ in terms of local G exactly:

$$\begin{aligned} V_i &= \Delta^{-1}[i] \cdot \mathcal{V}_i \cdot \Delta[i] \\ \Phi_i &= \Delta^{-1}[i] \cdot (\partial_{\tau_i} \Delta[i]) \end{aligned}$$

$$\Delta[j] = \frac{1}{1 - \det[\hat{G}[j^-, j]]} \left(1 - \hat{G}^k[j^-, j]\right)$$

Now we have a canonical but non polynomial theory!

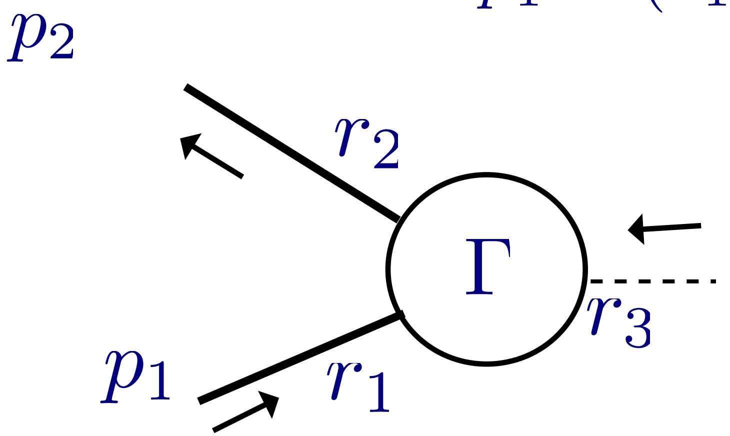
Schwinger Dyson vertex

Hubbard model
Schematic

$$\Gamma(r_1, r_2; r_3) = -\frac{\delta G^{-1}(r_1, r_2)}{\delta V(r_3)}$$

$$p_1 = (\vec{k}_1, \omega_1)$$

A vertex
function a la
Feynman Dyson



Bethe Salpeter Equation

$$\Gamma(p_1, p_2) = 1 + \sum_{p_3} I(\{p\})G(q)\Gamma(q, q + p_2 - p_1)G(q + P_2 - p_1)$$

Asymptotic Freedom of vertex implies

$$\lim_{\omega_n \to \infty} \Gamma(\vec{k}_1, \omega_1, \vec{k}_2, \omega_2) \to 1$$

Similarly: we can set up a set of eqns for tJ model using the exact EOM. We first need to invert the canonical equation and then take derivatives w.r.t. sources.

$$\frac{\delta}{\delta V}\mathcal{G}^{-1}$$

Sick vertex : grows with frequency

$$\frac{\delta}{\delta V}\hat{G}^{-1}$$

Healthy vertex satisfies Asymptotic Freedom

Exact expression for Greens Function in the ECQL. A strong coupling quantum liquid with no broken symmetries (non perturbative)

$\mathcal{G}(i,j) =$ Bare particle Greens fn $\quad \hat{G}(i,j) =$ Quasi particle Greens fn

$$\mathcal{G}(i,j) = (1-n/2)\ \hat{G}(i,j)$$

$$\boxed{\hat{G}^{-1}[k] = i\omega_k + \mu - \xi_0\ \varepsilon_k - \frac{1}{2}\sum_q \left(\varepsilon_q + \frac{1}{2} J_{k-q}\right)\ \hat{G}[q]\ \{\ \Gamma_s[q,k] - 3\ \Gamma_t[q,k]\}.}$$

$$\xi_0 \equiv \frac{1}{1-\frac{n}{2}}\{(1-\frac{n}{2})^2 + \langle \vec{S}_{\vec{0}} \cdot \vec{S}_{\vec{\eta}} \rangle + \frac{1}{4}(\langle n_{\vec{0}}\ n_{\vec{\eta}} \rangle - n^2)\}$$

Singlet and Triplet p-h vertices

Notice that dispersion involves exact spin charge correlations at nearest neighbour lengths scale. Due to AFM correlations get band reduction

$$m_k = k_B T \sum_{i\omega_k}\ e^{i\omega_k 0^+} \hat{G}[k, i\omega_k]$$

$$\frac{1}{N_s}\sum_{\vec{k}} m_k = \frac{n}{2-n}$$

Modified Pauli Principle for Quasiparticles
Leads to fractional charge interpretation
for the quasiparticles; and also to the violation of
Luttinger & Ward's sum rule for Fermi surface volume

Vertex equations

+ Stopping rule?

$$
\begin{aligned}
\Gamma_s[i,j;m]_1 &= \frac{1}{4}(n-2)^2 t[i,j]\chi_s[j,j,m] \\
\Gamma_s[i,j;m]_2 &= \frac{3}{8}(n-2)\ \lambda\ t[i,j]\left((n-2)\chi_t[i,i,j]\chi_s[j,j,m] - 2\Gamma_t[a,b,j]\left(\hat{G}[i,a]\chi_s[b,i,m] + \hat{G}[b,i]\chi_s[i,a,m]\right)\right.
\end{aligned}
$$

$$\Gamma_t[i,j;m]_1 = -\tfrac{1}{4}(n-2)^2\ \lambda\ t[i,j]\chi_t[j,j,m]$$

+....

$$\boxed{\lambda = \frac{1}{1-n}}$$

What are we perturbing in? Answer: emergent small parameter is Mott Hubbard hole density

Gutzwiller factors end up giving this inverse hole density factor.
Useful as a stopping criterion for hierarchy

Lesson from Bruekner's Nuclear matter: Small parameter is not the interaction constant but rather the particle density scaled by the scattering length cubed. This is a classic example of emergent small parameters in field theory.

To lowest order, we can set vertex to unity in the RHS.
Get large number of terms contributing to self energy.
GGG theory: numerical results later.

Use Ward identities for gauge invariance and Nozieres relations for enforcing rotation invariance

First Result

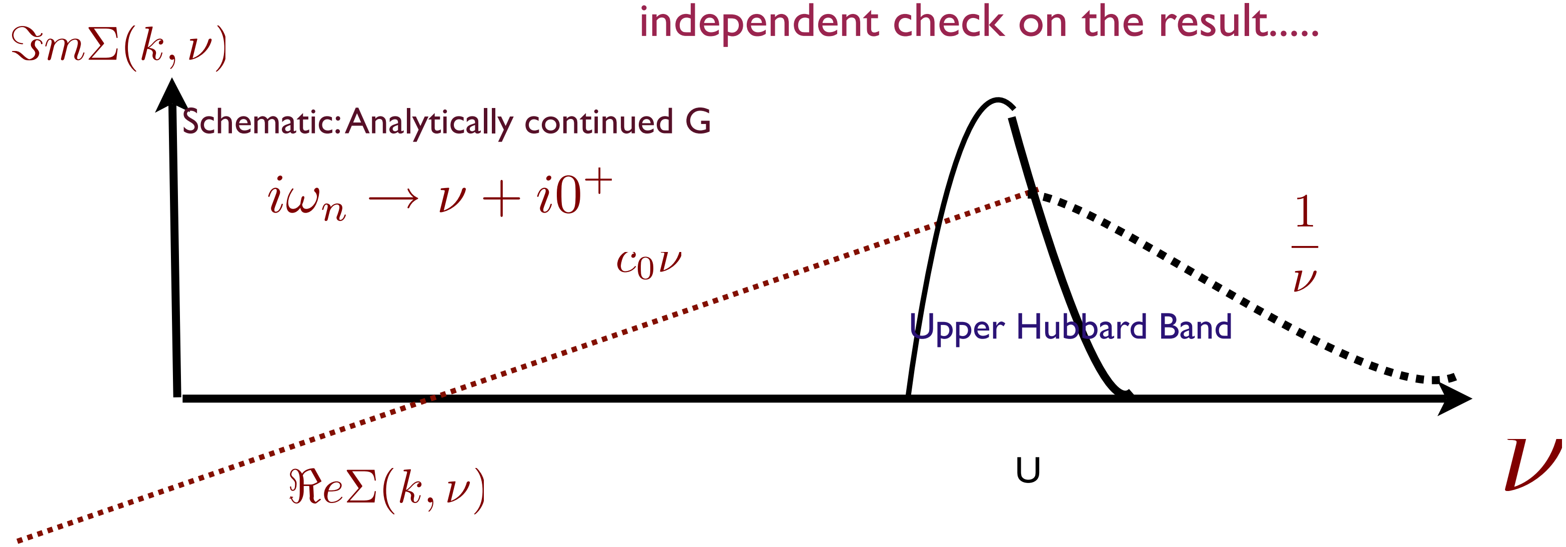
Luttinger Ward theorem is invalid in the ECQL phase, get a systematically larger FS

$$\boxed{\frac{1}{N_s}\sum_{\vec{k}}\theta(\hat{G}(\vec{k},0)) = \frac{n}{2-n}}$$

On shell Greens function is real and
LHS gives the volume where it is positive
New Sum rule for FS with a renormalized RHS.

$$\Sigma(\vec{k}, i\omega_n) \to -\frac{n}{2-n}\, i\omega_n$$

Appendix D discusses the origin of the failure of LW
Self energy in the extreme limit (U= infinity) has a pathological growth with frequency. Hence one can redo the LW argument and arrive at the same final answer as here- an independent check on the result.....



Luttinger Ward (& AGD) meet extreme correlations

Test case of Atomic limit where t=0 in Hubbard model

$$G_{\text{atomic}}(i\omega_n) = \frac{1-\frac{n}{2}}{i\omega_n+\mu} + \frac{\frac{n}{2}}{i\omega_n+\mu-U}, = \frac{1}{i\omega_n+\mu-\Sigma(i\omega_n)}, \quad \text{with}$$

$$\Sigma(i\omega_n) = U\frac{n}{2} + U^2 \frac{\frac{n}{2}(1-\frac{n}{2})}{i\omega_n+\mu-U(1-\frac{n}{2})}$$

$$\text{Weak Coupling HF limit} \qquad \omega_n \to \infty \qquad U \sim O(1) \qquad \frac{U}{\omega_n} \to 0$$

$$\text{Extreme Coupling HF limit} \qquad \omega_n \to \infty \qquad U \to \infty \qquad \frac{U}{\omega_n} \to \infty$$

$$\Sigma_{EC}(i\omega_n) \quad = c_0(i\omega_n+\mu)$$

$$\boxed{c_0 = -\frac{n}{2-n}}$$

For non zero k we expect, here c_0 fixes the asympt behaviour in EC limit

$$\boxed{\Sigma(\vec{k},z)/\lim_{U\to\infty} = c_0(z+\mu) + \Sigma_{\text{Regular}}(\vec{k},z)}$$

Where Σ_{Regular} goes as 1/z

Boundary terms cannot be thrown out in extreme correlation limit

$$n = 2\sum_k G(\vec{k}, i\omega_n)e^{i\omega_n \eta} = \frac{2}{N_s}\sum_{\vec{k}}\int_{-\infty}^{0}\frac{dx}{2\pi i}\left\{G(\vec{k}, x-i\eta) - G(\vec{k}, x+i\eta)\right\}.$$

$$G(\vec{k}, z) = 1/(z+\mu-\varepsilon_k - \Sigma(\vec{k}, z))$$

$$G(\vec{k}, z) = -\frac{d}{dz}\log G(\vec{k}, z) + G(\vec{k}, z)\frac{d}{dz}\Sigma(\vec{k}, z)$$

$$n = n_1 + n_2$$

$$n_1 = \frac{2}{N_s}\sum_{\vec{k}}\Theta(G(\vec{k}, 0))$$

$$n_2 = \frac{2}{N_s}\sum_{\vec{k}}\int_{-\infty}^{0}\frac{dx}{2\pi i}\left\{G(\vec{k}, x-i\eta)\frac{d}{dx}\Sigma(\vec{k}, x-i\eta) - G(\vec{k}, x+i\eta)\frac{d}{dx}\Sigma(\vec{k}, x+i\eta)\right\}$$

L-W argue that $n_2=0$.
By using integration by parts + LW Functional.

However, since Σ grows linearly with ω
(and G decays as $1/\omega$)

$$\int G\frac{d}{dx}\Sigma \neq -\int \Sigma\frac{d}{dx}G$$

Using correct large ω behaviour of Σ , we find instead

$$n_2 = c_0\, n + n_3$$
$$n_3 = 0$$

Therefore we get a different
Fermi Surface Sum Rule

$$\boxed{\frac{n}{1-\frac{n}{2}} = \frac{2}{N_s}\sum_{\vec{k}}\Theta(G(\vec{k}, 0))}$$

1.High T results of Rajiv Singh, Bill Putikka PRL (2006) show violations of LW Sum rule

2.Exact Diagonalization Prelovsek Kokalj

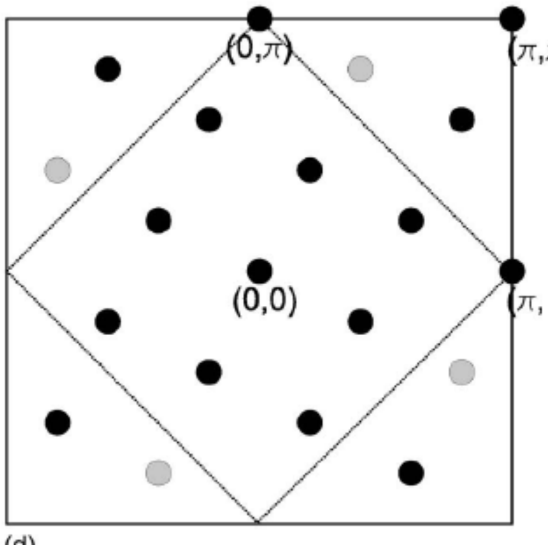
PHYSICAL REVIEW B **75**, 045111 (2007)

Luttinger sum rule for finite systems of correlated electrons

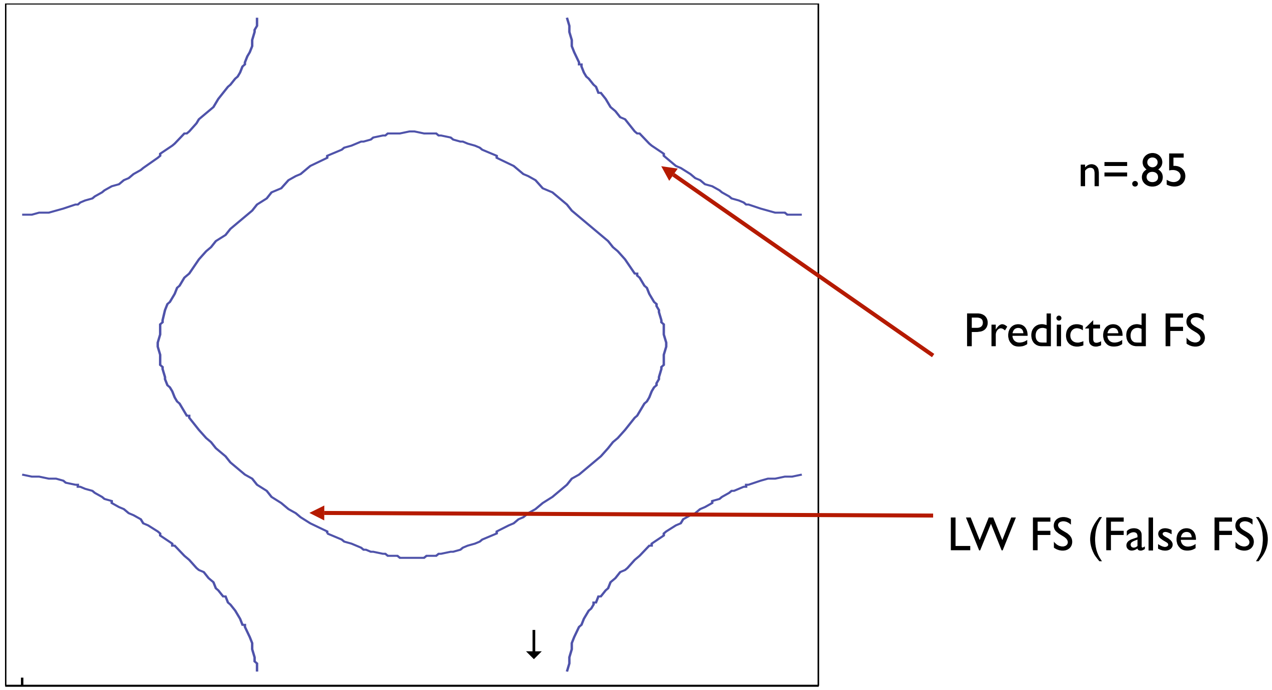
J. Kokalj[1] and P. Prelovšek[1,2]

$$N = \sum_{\mathbf{k}s, G_s(\mathbf{k},0)>0} 1,$$

$$G_s(\mathbf{k},\zeta) = \sum_m \frac{|\langle m_{N-1}|c_{\mathbf{k}s}|0_N\rangle|^2}{\zeta + \mu_N - (E_0^N - E_m^{N-1})} + \sum_l \frac{|\langle l_{N+1}|c^\dagger_{\mathbf{k}s}|0_N\rangle|^2}{\zeta + \mu_N - (E_l^{N+1} - E_0^N)}.$$

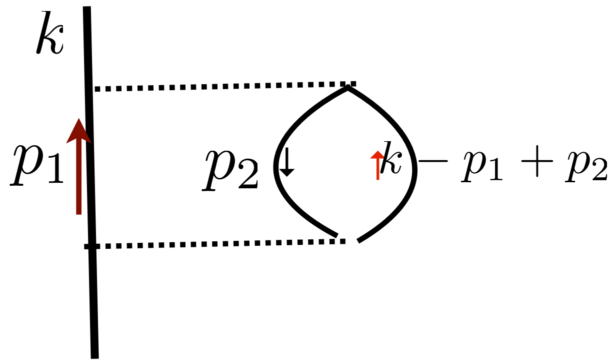


Luttinger volume for closed shell configuration of $N=18$ electrons on $N_0=20$ square lattice



Next we compare spectra for tJ model within GGG scheme and Hubbard (n=.9, U= 3 t)
GGG = skeleton graphs self consisted

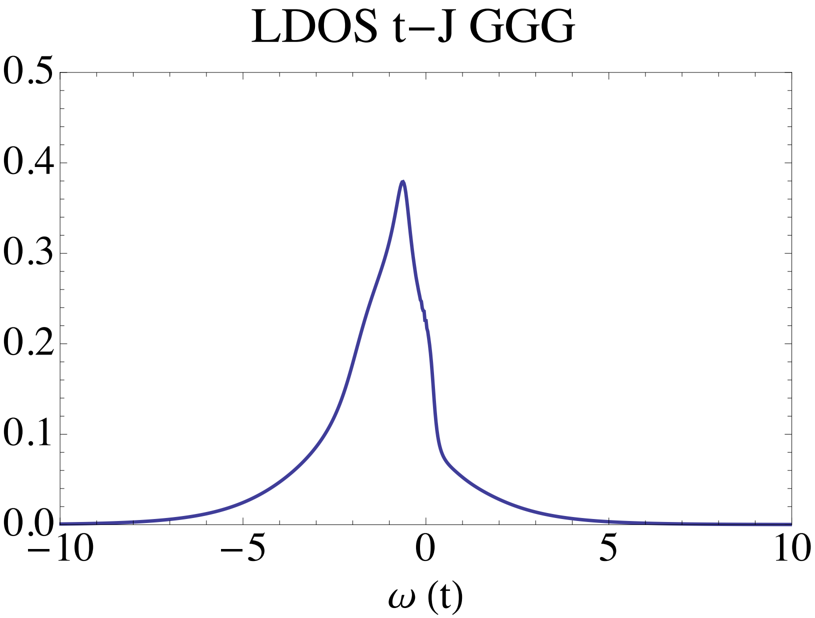
$$\Sigma(k) \sim U^2 \sum_{p_1,p_2} G(p_1)G(p_2)G(k-p_1+p_2)$$

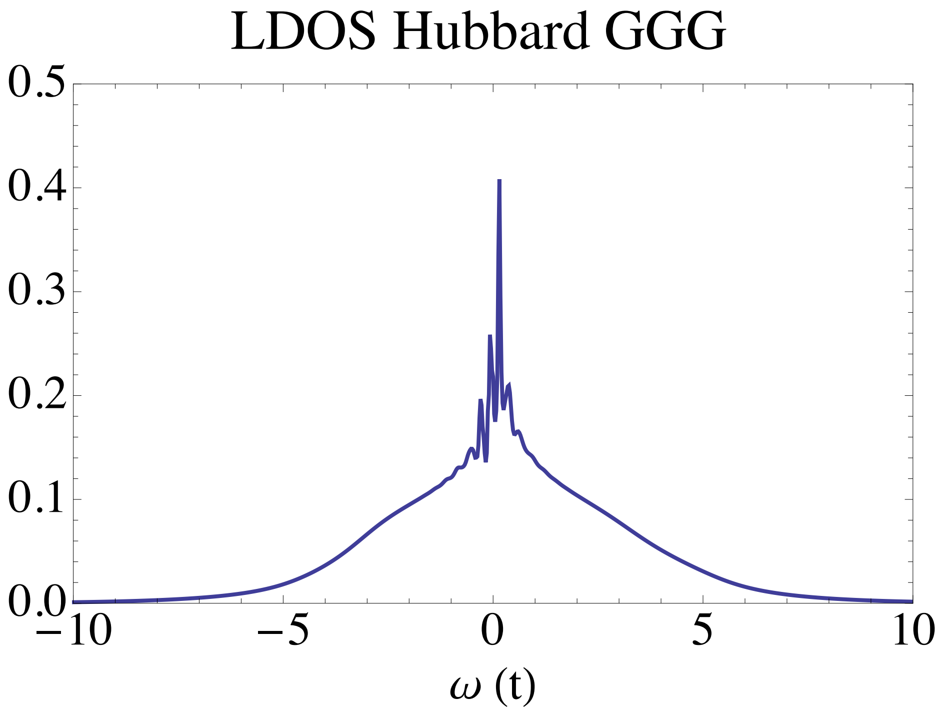


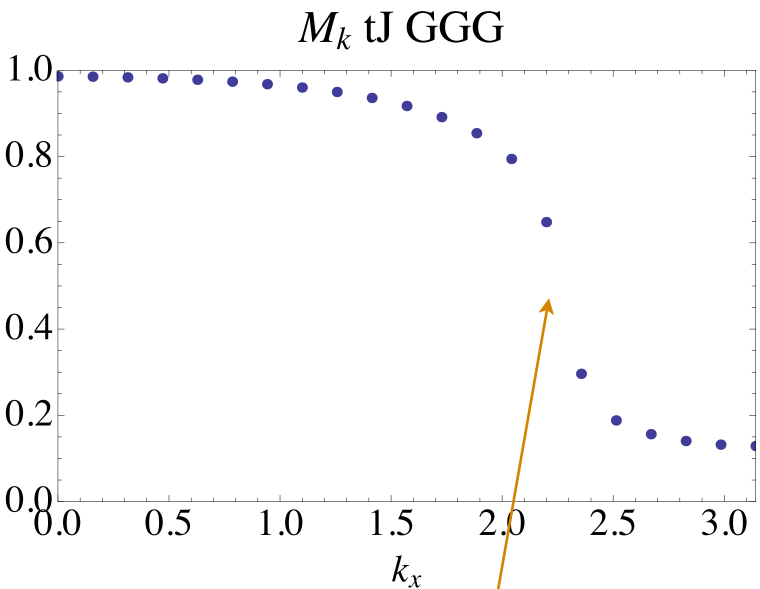
Daniel Hansen+ SS
unpublished

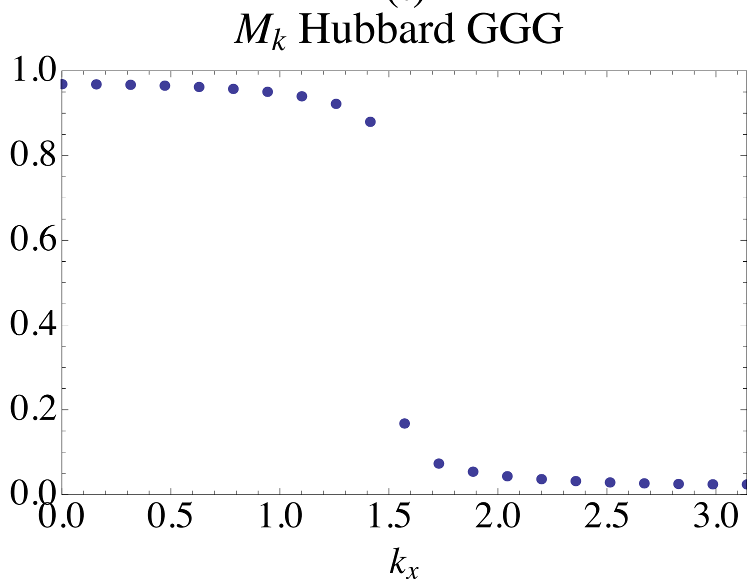
$$\delta S[k] = \frac{1}{2}\sum_q \left(\varepsilon_q + \frac{1}{2}J_{k-q}\right)\ \hat{G}[q]\ \{\ \Gamma_s[q,k] - 3\ \Gamma_t[q,k]\}.$$

$$\begin{aligned}
\Gamma_s[q,k] \ - \ 3\ \Gamma_t[q,k] = \\
& -\chi_1(q-k)(4 + 3\lambda j m_{\vec{\eta}}(1-\frac{n}{2})) \\
& -\chi_0(q-k)(2m_{\vec{\eta}}(1-\frac{n}{2})(1-3\lambda) + 4j(1-\frac{n}{2})^2 x_s\chi_{\mathrm{loc}}(8+3\lambda+\frac{3}{2}\lambda^2)) \\
& -\chi_0(q-k)(\varepsilon_k(1-\frac{n}{2})^2 x_s\chi_{\mathrm{loc}}(3\lambda-1+3n\lambda^2) + J_k(1-\frac{n}{2})m_{\vec{\eta}}3\lambda) \\
& -\chi_0(q-k)(\varepsilon_q(1-\frac{n}{2})^2(1+3\lambda+\frac{x_s\chi_{\mathrm{loc}}}{2}(1+6\lambda-3\lambda^2)) - 3\lambda m_{\vec{\eta}} J_q(1-\frac{n}{2})) \\
& -\chi_0(q-k)(m_{\vec{\eta}}\varepsilon_{q-k}(1-\frac{n}{2})(3\lambda-1) + \frac{J_{q-k}}{2}(1-\frac{n}{2})^2((1+3\lambda)+3x_s\chi_{\mathrm{loc}}(\frac{2n-3}{2}\lambda^2-8))) \\
& -\sum_r G[r]G[r+q-k]\varepsilon_{r-q}(-2j+\frac{m_{\vec{\eta}}}{2}(1-\frac{n}{2})(1+3\lambda(5-n))) \\
& -\sum_r G[r]G[r+q-k]\varepsilon_{r+k}(2m_{\vec{\eta}}(1-\frac{n}{2}))
\end{aligned}$$



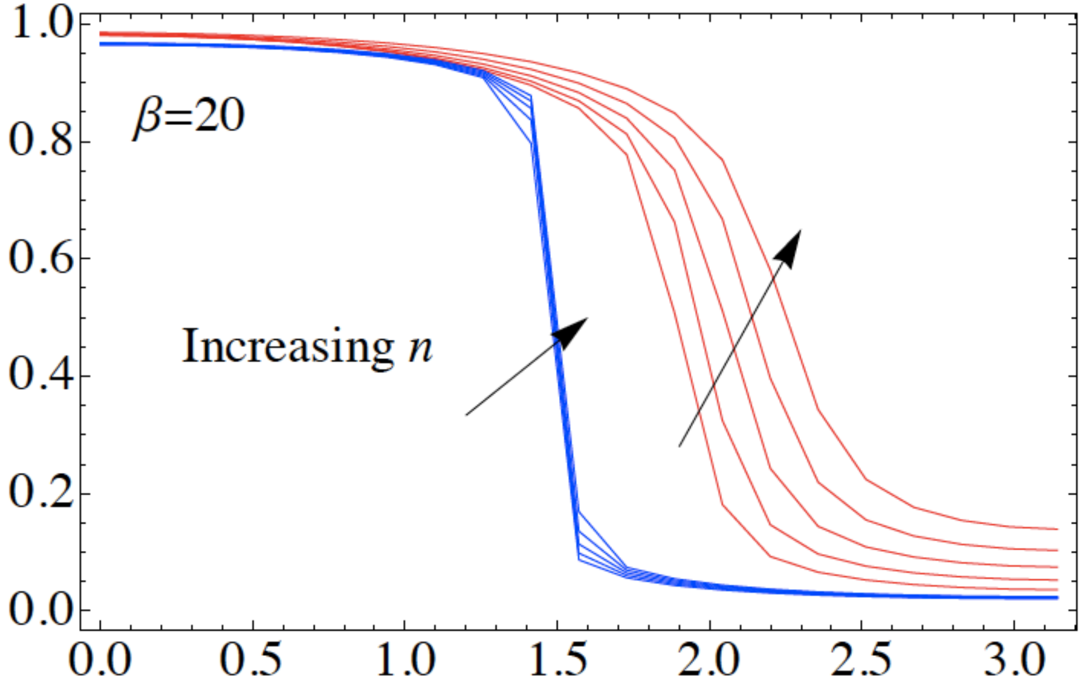




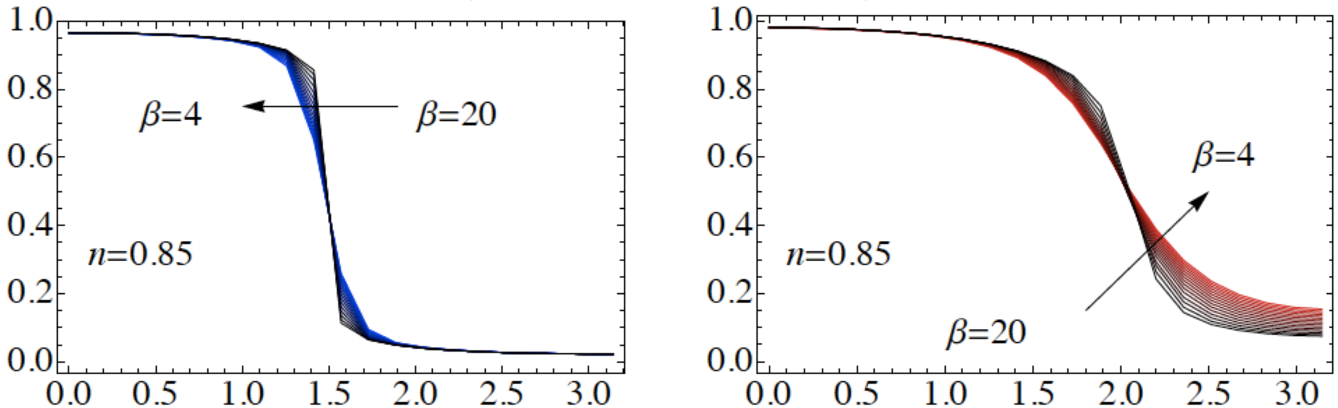


Notice absence of jump

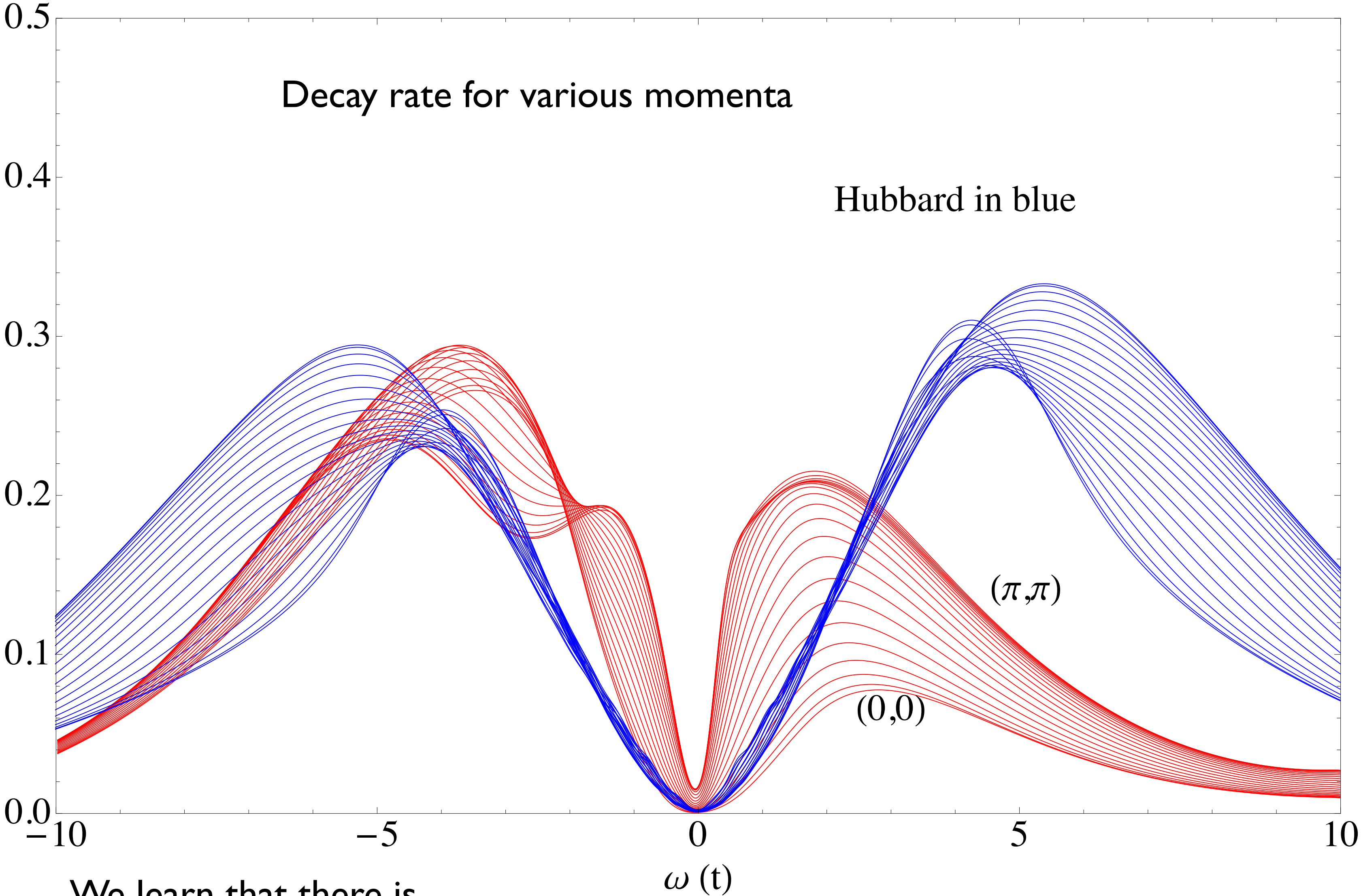
Nodal m_k



Temperature dependence of M_k
(Dark colors are colder)



ρ_Σ vs ω for k along (11) t−J GGG



We learn that there is strong k dependence in tJ unlike Hubbard

Define Q(k,T), the "quality" factor of peak

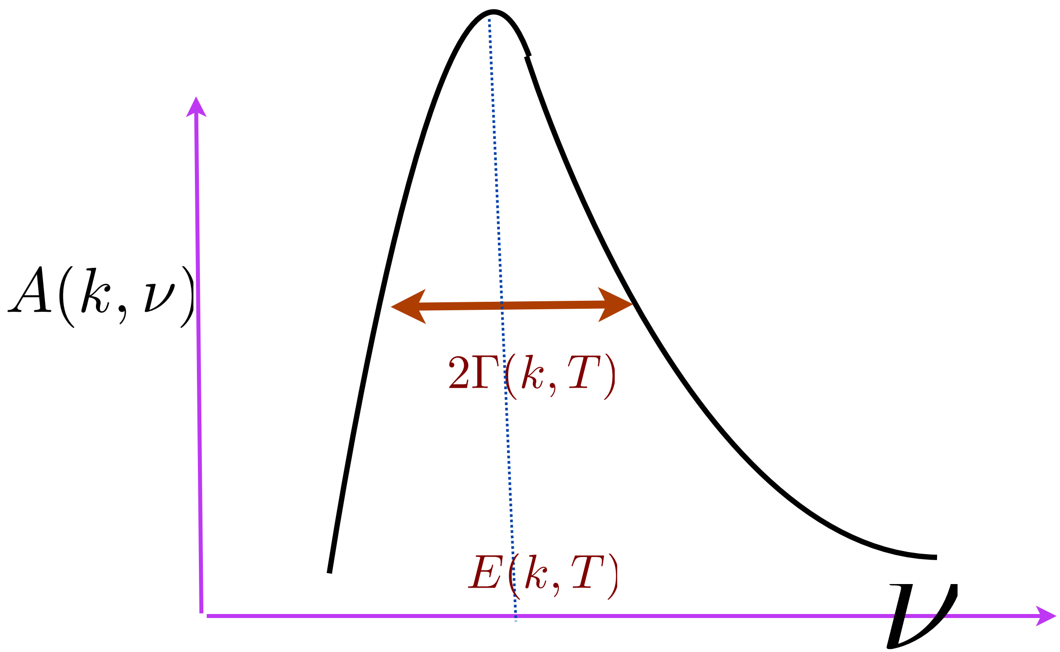
A is spectral function

$$A(k,\nu) = \frac{\Im m\ \Sigma(k,\nu)}{[\nu - \xi_0\ \varepsilon(k)\Re e\ \Sigma(k,\nu)\ ]^2 + [\Im m\ \Sigma(k,\nu)\ ]^2}$$

$$\boxed{E(k) = \xi_0\ \varepsilon(k) + \Re e\ \Sigma(k, E(k))}$$

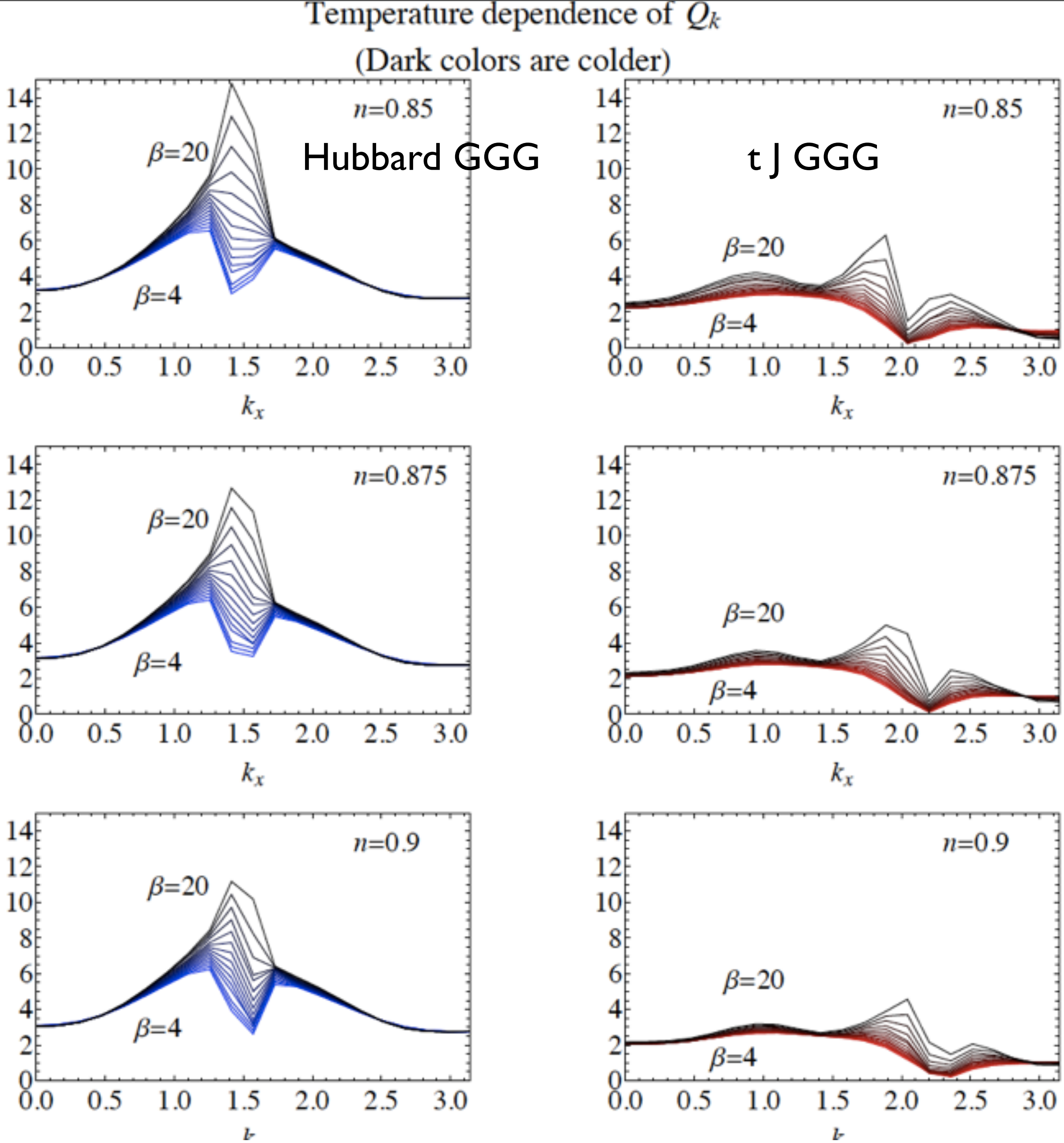
Quasiparticle energy E(k) definition, its width Γ(k,T) and its quality factor Q(k,T)

$$Q(k,T) = \frac{E(k)}{\Gamma(k,T)}$$

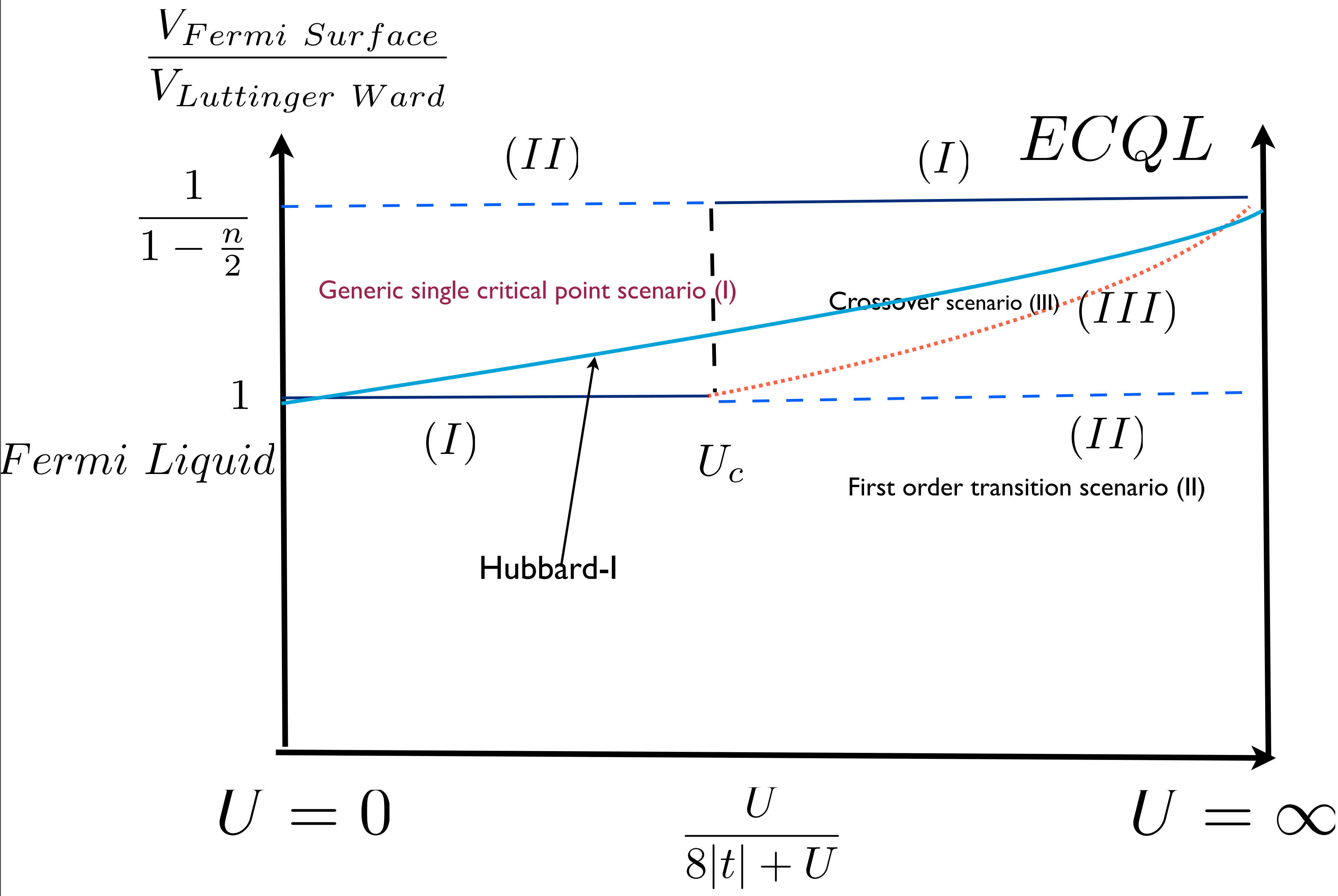


Expect large Q(k_f,0) in Fermi liquids.

$$\Gamma(k,T) = \sqrt{\Gamma(k,0)^2 + c^2(k_B T)^2}$$



- tJ show very poor Q compared to Hubbard
- Inverted peak structure near kF, with low T Q factors being larger than high T ones,
- Unlike Hubbard model Considerable T dependence away from k_F



$\frac{V_{Fermi\ Surface}}{V_{Luttinger\ Ward}}$
$\frac{1}{1-\frac{n}{2}}$
(II)
(I)
$ECQL$
Generic single critical point scenario (I)
Crossover scenario (III)
(III)
1
$Fermi\ Liquid$
(I)
U_c
(II)
First order transition scenario (II)
Hubbard-I
$U = 0$
$\frac{U}{8|t|+U}$
$U = \infty$

Summary and open Questions

- Non canonical Field theories using Schwinger's ideas + crucial insight re asymptotic freedom of vertices. Factoring in time space
- We find by a self consistent theory, ECQL, i.e. a strong coupling quantum liquid phase of the tJ model found with large FS.
    - Question: Is this the unique liquid phase for the tJ model or can we have other liquids states (satisfying LWT)?
- Preliminary result : Superconducting instability has a similar form to RVB d-wave, but very small Tc.
- Connection with experimental systems?
    - Does the tJ model really describe High Tc systems? Or is Hubbard more appropriate?
    - Interesting and probing questions are emerging re ARPES line width:
    - Is $\Gamma(k)$ a minimum at "FS" - preliminary answers confusing