Continuous time Quantum Monte Carlo methods for electron-phonon interactions in correlated electron systems.

F.F. Assaad (KITP, 13th August 2009)

Motivation: Methods to tackle electron-phonon problems (retarded interactions)

Outline

- Weak coupling CT-QMC (Rubtsov et al. PRB 05).
- Retarded interactions: phonon degrees of freedom.
- Application to the 1D quarter filled Holstein model.
- Conclusions.

F.F. Assaad and T.C. Lang
Phys. Rev. B 76, 035116 (2007), Phys. Rev. B 78 155124 (2008)

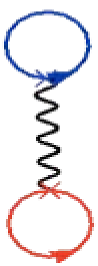
I. Weak coupling CT-QMC for the SIAM.

$$S = \underbrace{-\int d\tau\, d\tau'\, d_\sigma^+(\tau)\, \mathcal{G}_0^{-1}(\tau-\tau')\, d_\sigma(\tau')}_{S_0} + U\int_0^\beta d\tau\ \underbrace{d_\uparrow^+(\tau)\, d_\uparrow(\tau)}_{n_\uparrow(\tau)}\, d_\downarrow^+(\tau)\, d_\downarrow(\tau)$$

Dyson. Expansion around U=0.

$$\frac{\mathrm{Tr}\left[e^{-\beta H}\right]}{\mathrm{Tr}\left[e^{-\beta H_0}\right]} = \sum_n \int_0^\beta d\tau_1 \cdots \int_0^{\tau_{n-1}} d\tau_n\, (-U)^n \ \left\langle n_\uparrow(\tau_1) n_\downarrow(\tau_1) \cdots n_\uparrow(\tau_n) n_\downarrow(\tau_n) \right\rangle_0$$

Wick

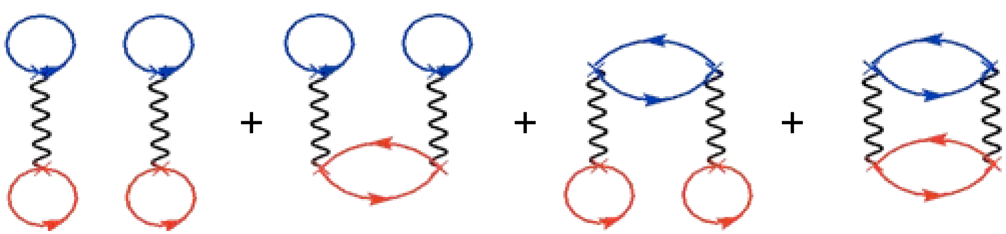
n=1 

$G_0{}^\uparrow$

$G_0{}^\downarrow$

$$\mathrm{U} \quad = -U \det\begin{pmatrix} G_0{}^\uparrow(\tau_1,\tau_1) & 0 \\ 0 & G_0{}^\downarrow(\tau_1,\tau_1) \end{pmatrix} \equiv -U \det\left[M_1(\tau_1)\right]$$

$$G_0{}^\sigma(\tau_2,\tau_1) = \left\langle T\, \hat{d}_\sigma^+(\tau_2) \hat{d}_\sigma(\tau_1) \right\rangle_0$$

n=2 

$$= U^2 \det\left[M_2(\tau_1,\tau_2)\right]$$

$$\frac{\mathrm{Tr}\left[e^{-\beta H}\right]}{\mathrm{Tr}\left[e^{-\beta H_0}\right]} = \underbrace{\sum_n \int_0^{\beta} d\tau_1 \cdots \int_0^{\tau_{n-1}} d\tau_n}_{\textit{Sum}\ \text{with Monte Carlo}} \underbrace{(-U)^n \det\left[M_n\left(\tau_1,\cdots,\tau_n\right)\right]}_{\text{Weight}}$$

Weight / Sign.

➢ $$H_U \rightarrow \frac{U}{2}\sum_{s=\pm 1}\left(n_{\uparrow}^{d} - [1/2 - s\delta]\right)\left(n_{\downarrow}^{d} - [1/2 + s\delta]\right) = -\frac{K}{2\beta}\sum_s e^{s\alpha\left(n_{\uparrow}^{d} - n_{\downarrow}^{d}\right)}$$

$$K = U\beta(\delta^2 - 1/4), \ \cosh(\alpha) - 1 = \frac{1}{2(\delta^2 - 1/4)}, \qquad \delta > 1/2$$

→ New dynamical variable s. Exact mapping onto CT-Hirsch-Fye (K. Mikelsons et al. preprint) (Rombouts et al. PRL 99, Gull et. al EPL 08)

→Sign problem behaves as in Hirsch-Fye. (Absent for one-dimensional chains, particle-hole symmetry, impurity models)

$$\frac{\mathrm{Tr}\left[e^{-\beta H}\right]}{\mathrm{Tr}\left[e^{-\beta H_0}\right]} = \underbrace{\sum_n \int_0^\beta d\tau_1 \cdots \int_0^{\tau_{n-1}} d\tau_n}_{\textit{Sum} \text{ with Monte Carlo}} \underbrace{(-U)^n \det\left[M_n(\tau_1,\cdots,\tau_n)\right]}_{\text{Weight}}$$

Weight / Sign.

- $$H_U \rightarrow \frac{U}{2}\sum_{s=\pm 1}\left(n_\uparrow{}^d - [1/2 - s\delta]\right)\left(n_\downarrow{}^d - [1/2 + s\delta]\right) = -\frac{K}{2\beta}\sum_s e^{s\alpha\left(n_\uparrow{}^d - n_\downarrow{}^d\right)}$$

$$K = U\beta(\delta^2 - 1/4), \ \cosh(\alpha) - 1 = \frac{1}{2(\delta^2 - 1/4)}, \qquad \delta > 1/2$$

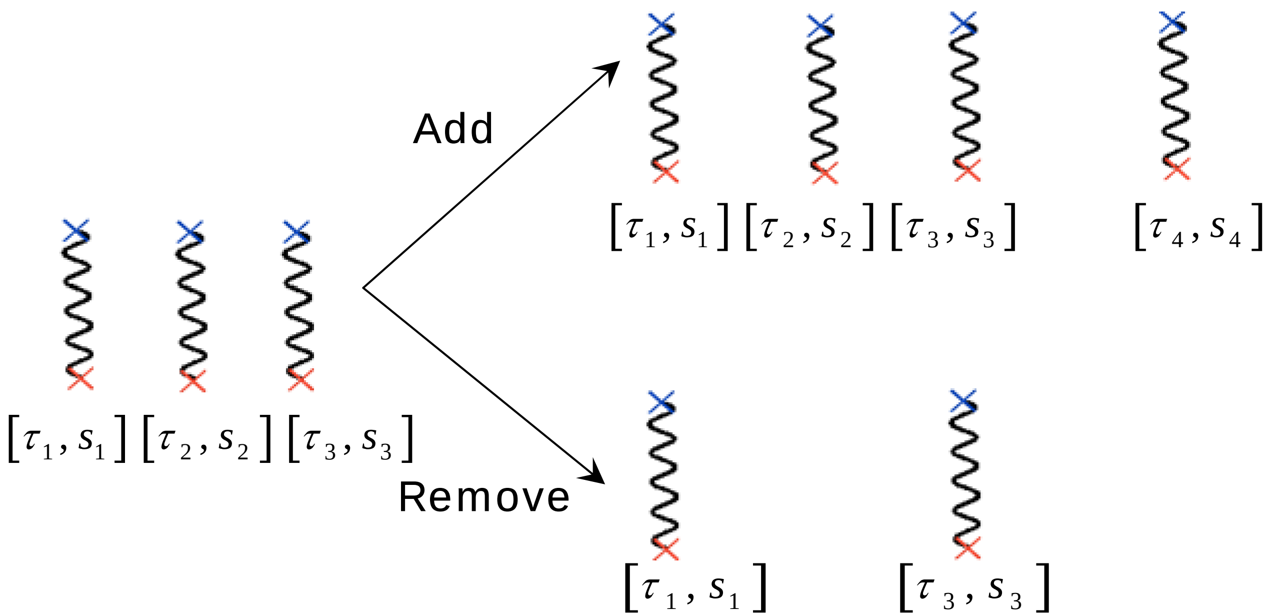
- $$H_U = U\left(n_\uparrow{}^d - [1/2 - \delta]\right)\left(n_\downarrow{}^d - [1/2 + \delta]\right) + \underbrace{U\delta(n_\uparrow{}^d - n_\downarrow{}^d)}_{\text{Absorb in } H_0}$$

- Particle-Hole symmetry $\delta = 0$ and only even powers of n occur in expansion.

$$\frac{\mathrm{Tr}\left[e^{-\beta H}\right]}{\mathrm{Tr}\left[e^{-\beta H_0}\right]} = \underbrace{\sum_n \int_0^\beta d\tau_1 \sum_{s_1} \cdots \int_0^{\tau_{n-1}} d\tau_n \sum_{s_n}}_{\textit{Sum}\text{ with Monte Carlo}} \underbrace{\left(-\frac{U}{2}\right)^n \det\left[M_n\left(\tau_1, s_1 \cdots, \tau_n, s_n\right)\right]}_{\text{Weight}}$$

Sampling.

Configuration C: set of n-vertices at imaginary times $[\tau_1, s_1][\tau_2, s_2]\cdots,[\tau_n, s_n]$



$$\frac{\mathrm{Tr}\left[e^{-\beta H}\right]}{\mathrm{Tr}\left[e^{-\beta H_0}\right]} = \underbrace{\sum_n \int_0^\beta d\tau_1 \sum_{s_1} \cdots \int_0^{\tau_{n-1}} d\tau_n \sum_{s_n}}_{\textit{Sum}\text{ with Monte Carlo}} \underbrace{\left(-\frac{U}{2}\right)^n \det\left[M_n\left(\tau_1, s_1 \cdots, \tau_n, s_n\right)\right]}_{\text{Weight}}$$

Measurements.

$$G^\sigma{}_C(\tau,\tau') \equiv \frac{\left\langle T\ H_U\left[\tau_1, s_1\right] \cdots H_U\left[\tau_n, s_n\right]\ \hat{d}^+_\sigma(\tau)\hat{d}_\sigma(\tau')\right\rangle_0}{\left\langle T\ H_U\left[\tau_1, s_1\right] \cdots H_U\left[\tau_n, s_n\right]\right\rangle_0} = G^\sigma{}_0(\tau,\tau') - \sum_{\alpha,\beta=1}^{n} G^\sigma{}_0(\tau,\tau_\alpha) \left(M^\sigma{}_n{}^{-1}\right)_{\alpha\beta} G^\sigma{}_0(\tau_\beta,\tau')$$

Wick theorem applies for each configuration C of vertices.

Direct calculation of Matsubara Green functions.

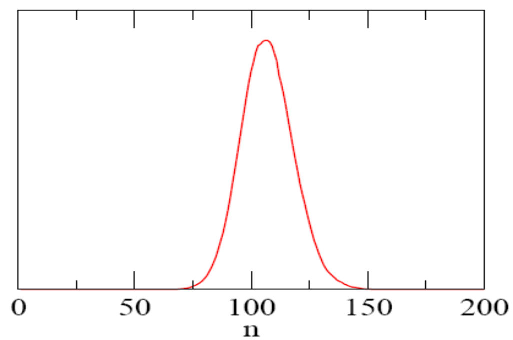
$$G^\sigma{}_C(i\omega_m) = G^\sigma{}_0(i\omega_m) - G^\sigma{}_0(i\omega_m) \sum_{\alpha,\beta=1}^{n} e^{-i\omega_m \tau_\alpha} \left(M^\sigma{}_n{}^{-1}\right)_{\alpha\beta} G^\sigma{}_0(\tau_\beta, 0)$$

$$\frac{\mathrm{Tr}\left[e^{-\beta H}\right]}{\mathrm{Tr}\left[e^{-\beta H_0}\right]} = \underbrace{\sum_n \int_0^\beta d\tau_1 \sum_{s_1} \cdots \int_0^{\tau_{n-1}} d\tau_n \sum_{s_n}}_{\textit{Sum}\text{ with Monte Carlo}} \underbrace{\left(-\frac{U}{2}\right)^n \det\left[M_n\left(\tau_1, s_1 \cdots, \tau_n, s_n\right)\right]}_{\text{Weight}}$$

Average Expansion parameter.

$$\langle n \rangle = -\beta U \left\langle \left(n^d_\uparrow - 1/2\right)\left(n^d_\downarrow - 1/2\right) - \delta^2 \right\rangle$$

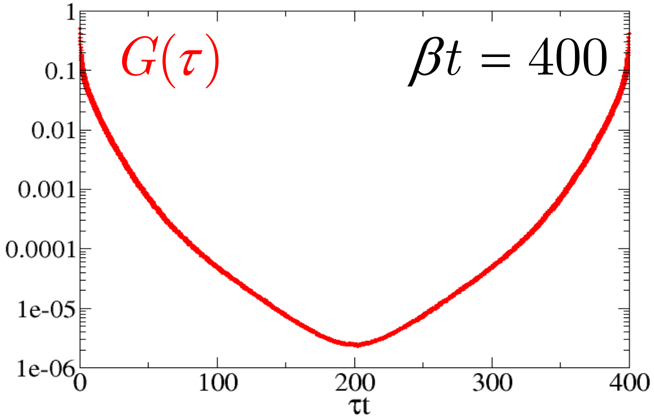
- CPU time scales as $\langle n \rangle^3$ → same scaling as Hirsch-Fye.
- $\langle n \rangle$ is minimal at particle-hole symmetric point, $\delta = 0$



Histogram of expansion parameter.

Examples.

a) Particle-hole symmetric Anderson Model, U/t=4.

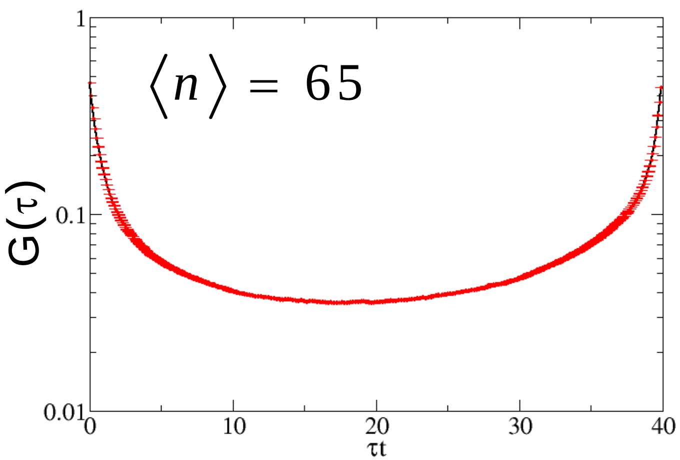


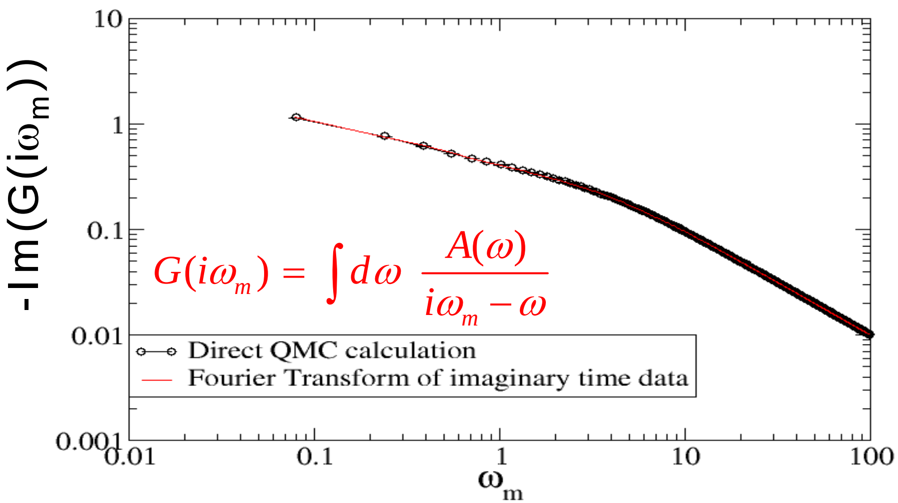
$\langle n \rangle = 270$

Hirsch-Fye: $L_{\mathrm{Trot}} = 400/0.2 \quad (\Delta \tau t = 0.2)$

Speedup: $(2000/270)^3 \approx 400$

b) Off particle-hole Symmetry, U/t=4 βt=40.





Speedup $(200/65)^3 \approx 30$

Direct calculation of $G(i\omega_m)$ is possible.

Continuous time Quantum Monte Carlo methods for electron-phonon interactions in correlated electron systems.

F.F. Assaad (KITP, 13th August 2009)

Motivation: Methods to tackle electron-phonon problems (retarded interactions)

Outline

- Weak coupling CT-QMC (Rubtsov et al. PRB 05).
- Retarded interactions: phonon degrees of freedom.
  (Hybridization expansion Werner & Millis PRL 99 07)
- Application to the 1D quarter filled Holstein model.
- Conclusions.

F.F. Assaad and T.C. Lang
Phys. Rev. B 76, 035116 (2007), Phys. Rev. B 78 155124 (2008)

II) Phonons. Integrate out phonons in favor of a retarded interaction.

Hubbard-Holstein:

$$\hat{H} = \sum_{i,j,\sigma} t_{i,j}\, \hat{c}^{+}_{i,\sigma}\hat{c}_{j,\sigma} + U\sum_{i}\hat{n}_{i,\uparrow}\hat{n}_{i,\downarrow} + g\sum_{i}\hat{Q}_i(\hat{n}_i - 1) + \sum_{i}\frac{\hat{P}_i^2}{2M} + \frac{k}{2}\hat{Q}_i^2$$

Integrate out the phonons

$$Z = \int\left[dc^{+}dc\right]\exp\left[-S_0 - U\int_0^{\beta} d\tau\; n_{i\uparrow}(\tau)n_{i\downarrow}(\tau) + \int_0^{\beta} d\tau\int_0^{\beta} d\tau' \sum_{i,j}[n_i(\tau)-1]D^0(i-j,\tau-\tau')[n_j(\tau')-1]\right]$$

$$D^0(i-j,\tau-\tau') = \delta_{i,j}\frac{g^2}{2k}P(\tau-\tau')$$

$$P(\tau) = \frac{\omega_0}{2(1-e^{-\beta\omega_0})}\left[e^{-|\tau|\omega_0} + e^{-(\beta-|\tau|)\omega_0}\right], \quad \omega_0 = \sqrt{k/M}$$

Attractive, retarded interaction (time scale $1/\omega_0$).

Antiadiabatic limit: $\lim_{\omega_0\to\infty} P(\tau) = \delta(\tau)$ → Attractive Hubbard.

II) Phonons. Integrate out phonons in favor of a retarded interaction.

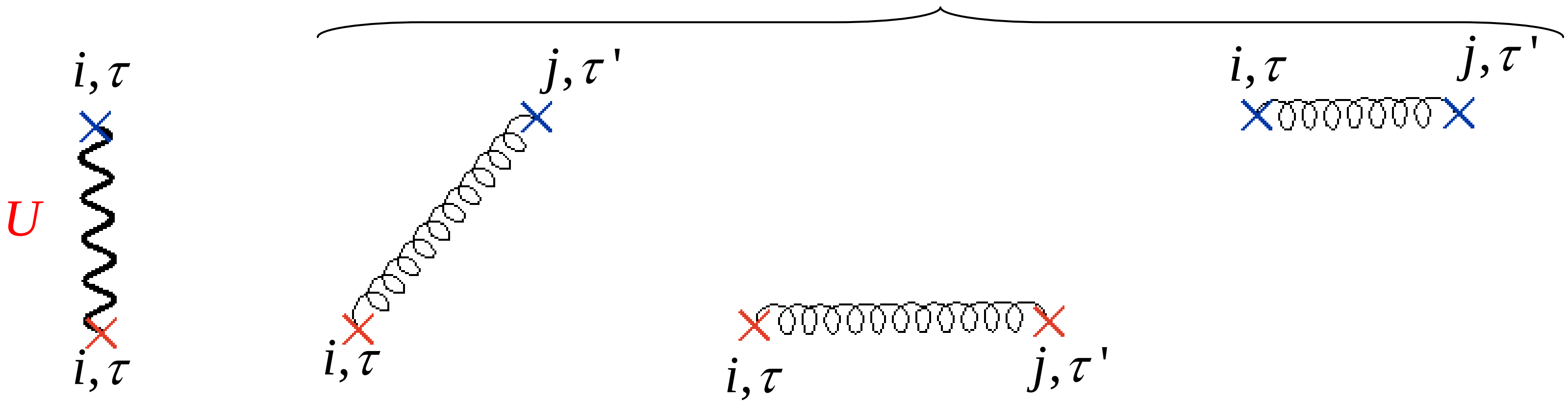
$$Z = \int \left[dc^{+} dc \right] \exp\left[-S_0 - U \int_0^{\beta} d\tau \; n_{i\uparrow}(\tau) n_{i\downarrow}(\tau) \; + \int_0^{\beta} d\tau \int_0^{\beta} d\tau' \sum_{i,j} [n_i(\tau) - 1] D^0(i-j, \tau - \tau') [n_j(\tau') - 1] \right]$$

QMC: Expand both in Hubbard and retarded phonon interaction.

Vertices:

Hubbard.

Phonon. $D^0(i-j, \tau-\tau')$



Continuous time Quantum Monte Carlo methods for electron-phonon interactions in correlated electron systems.

F.F. Assaad (KITP, 13th August 2009)

Motivation: Methods to tackle electron-phonon problems (retarded interactions)

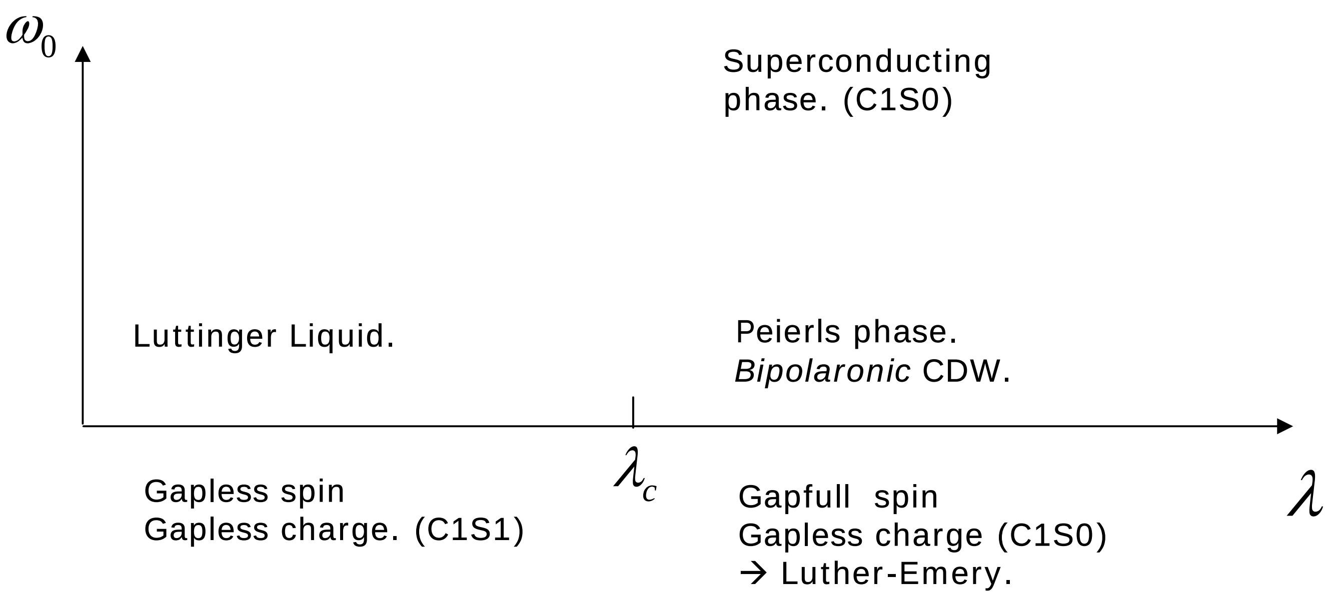
Outline

- Weak coupling CT-QMC (Rubtsov et al. PRB 05).
- Retarded interactions: phonon degrees of freedom.
  (Hybridization expansion Werner & Millis PRL 99 07)
- Application to the 1D quarter filled Holstein model.
- Conclusions.

F.F. Assaad and T.C. Lang
Phys. Rev. B 76, 035116 (2007), Phys. Rev. B 78 155124 (2008)

One-dimensional quarter filled Holstein model.

$$\hat{H} = \sum_{k,\sigma} \varepsilon(k)\hat{c}^{+}_{k,\sigma}\hat{c}_{k,\sigma} + g\sum_{i}\hat{Q}_i(\hat{n}_i - 1) + \sum_{i}\frac{\hat{P}_i^2}{2M} + \frac{k}{2}\hat{Q}_i^2$$



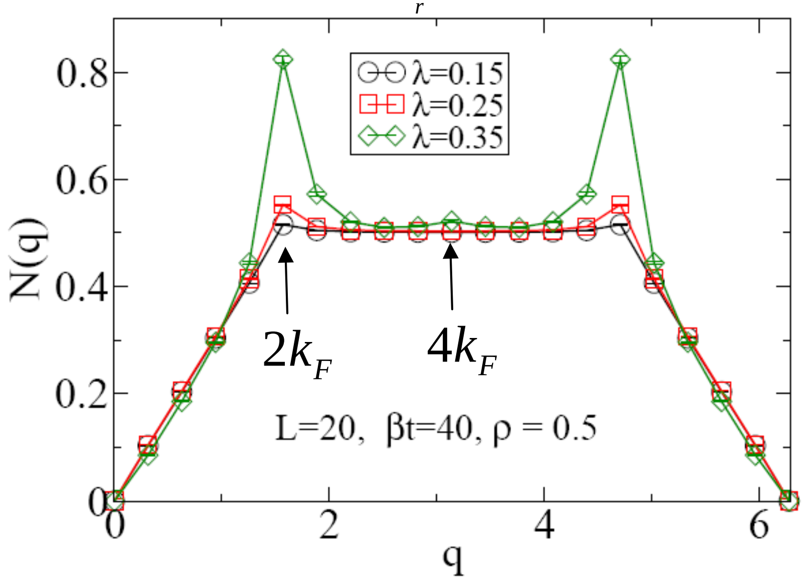
$\{\Sigma(i\omega_m) =$  Flat band width W → $\frac{m^*}{m} = 1 + \lambda, \quad \lambda = \frac{g^2}{2k}\frac{2}{W}\}$

Obtained from:

- Static and dynamical spin and charge structure factors, and optical conductivity (Lattice simulations; L=20, 28, T/t=1/40).
- Temperature dependence of the single particle spectral function (CDMFT, L_c=8-12).

Static properties @ ω_0=0.1t as a function of λ

Charge $N(q) = \sum_r e^{iqr} \langle \hat{n}(r)\hat{n}(0) \rangle$

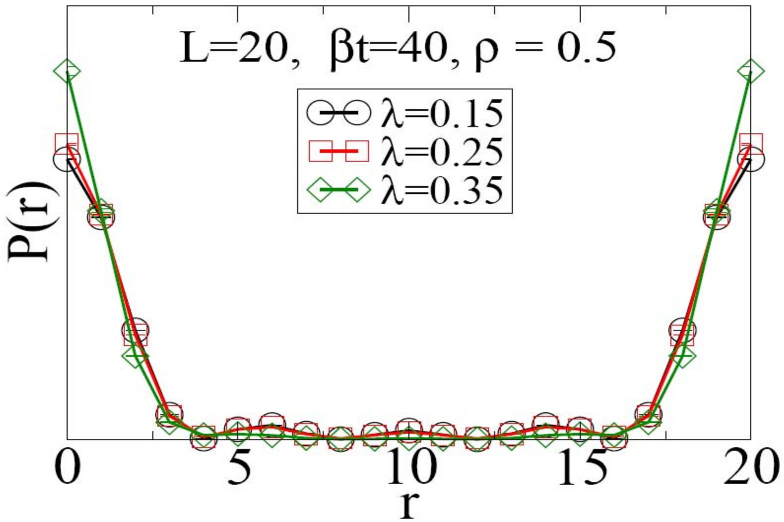


Dominant $2k_F$ charge correlations, at $\lambda \sim 0.35$

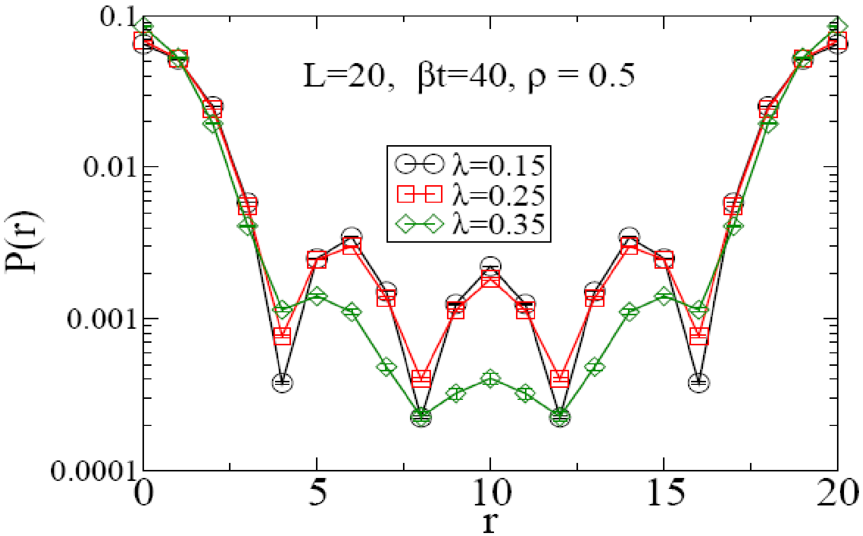
Luttinger Liquid: $\langle n(r)n(0) \rangle = \frac{K_\rho}{(\pi r)^2} + A_1 \cos(2k_f) r^{-(1+K_\rho)} + \cdots$

Static properties @ ω_0=0.1t as a function of λ

Pairing $P(r) = \left\langle \hat{\Delta}^\dagger(r)\hat{\Delta}(0)\right\rangle, \quad \hat{\Delta}^\dagger(r) = \hat{c}^\dagger_{r,\uparrow}\hat{c}^\dagger_{r,\downarrow}$



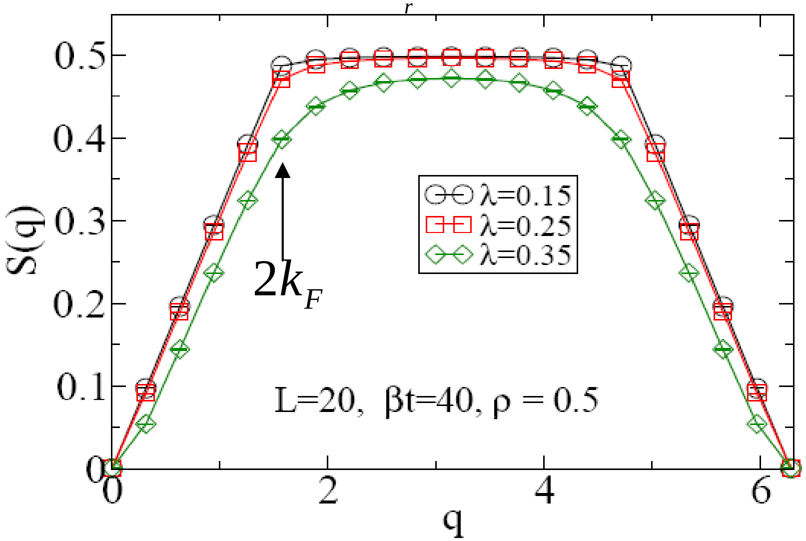
Short ranged pairing correlations grow → Two electrons with opposite spin share the same potential well (Bipolarons).



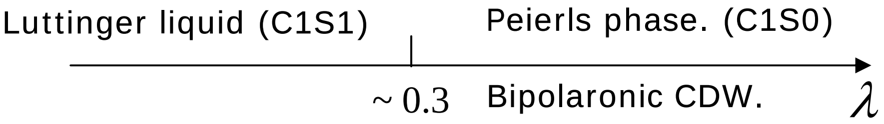
Long range pairing correlations drop → Bipolarons tend to localize.

Static properties @ ω_0=0.1t as a function of λ

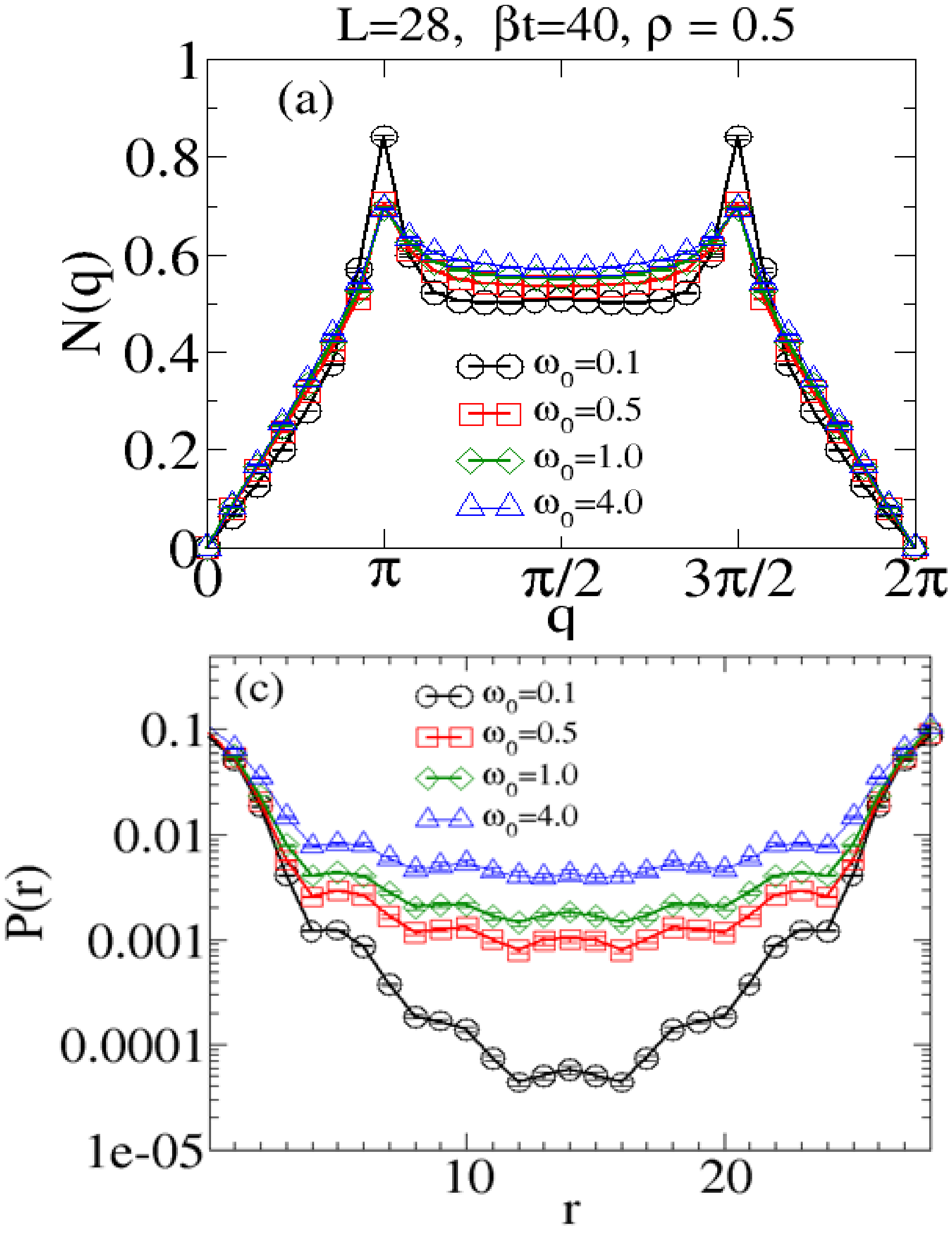
Spin $S(q) = \sum_r e^{iqr} \left\langle \hat{S}_z(r)\,\hat{S}_z(0) \right\rangle$



Pairing suppresses spin response.



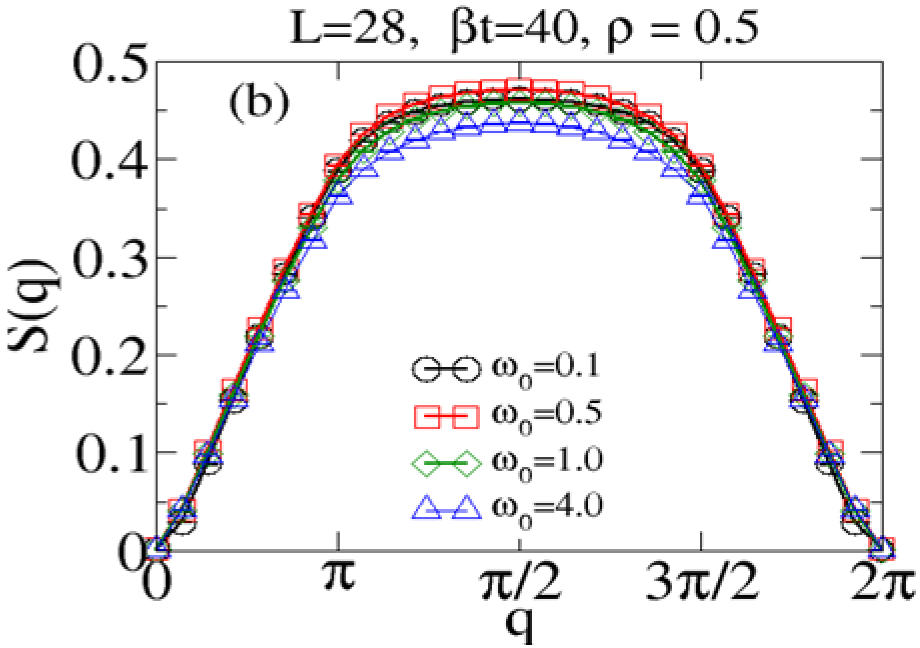
Static properties @ $\lambda = 0.35$ as a function of ω_0



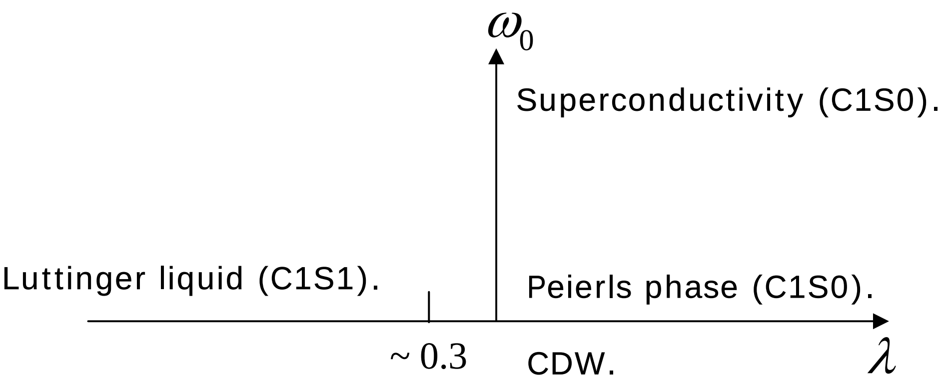
$2k_f$ charge correlations are suppressed

Pairing correlations are enhanced.

Static properties @ $\lambda = 0.35$ as a function of ω_0



Spin remains gapped.

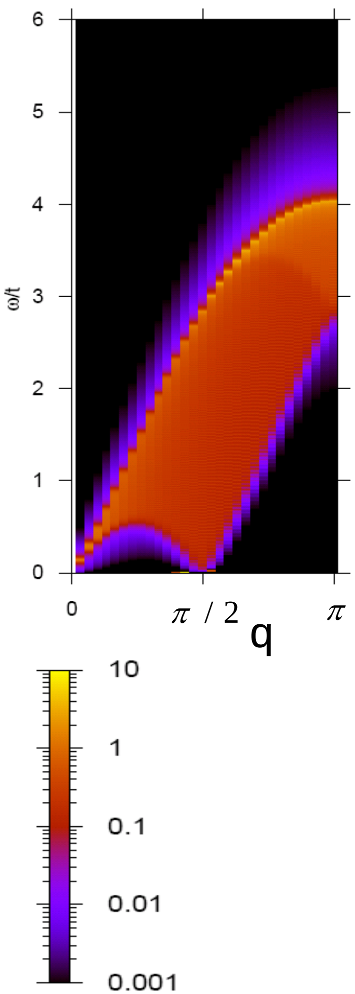


Charge dynamical structure factor. Lattice simulations. λ=0.35

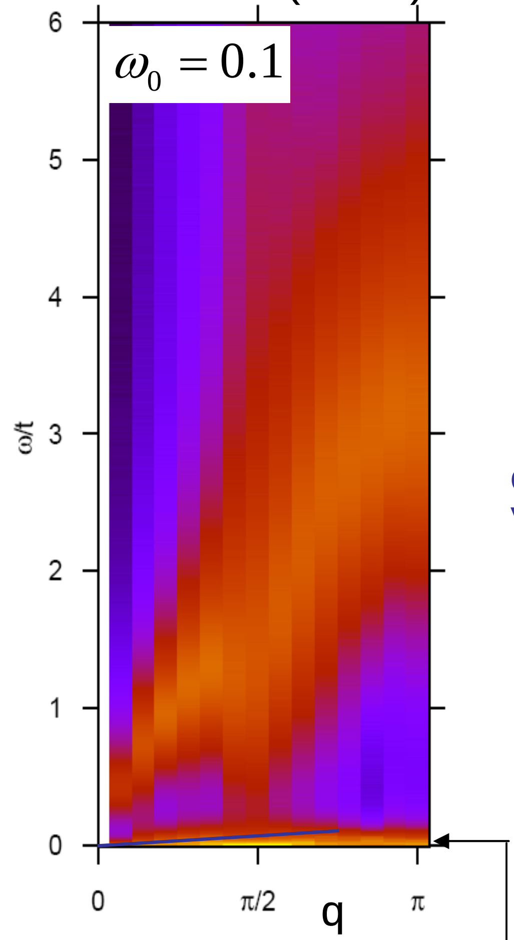
$$N(q,\omega) = \frac{1}{Z}\sum_{n,m} e^{-\beta E_m} \left|\langle n|\hat{n}(q)|m\rangle\right|^2 \delta(E_n - E_m - \omega)$$

$\beta t = 40, \ \rho = 0.5$

$\lambda = 0$

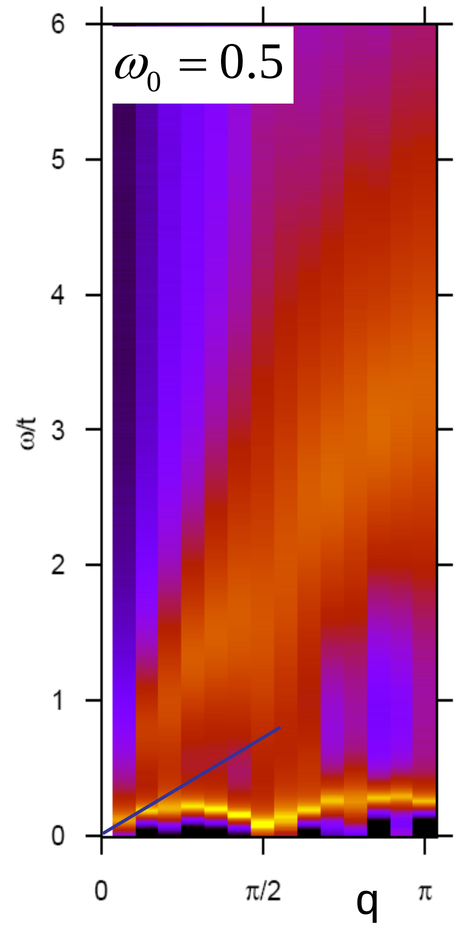


Peierls (CDW)



Charge Velocity.

Superconducting.



Piling up of spectral weight at $2k_f$. Slow dynamics of the bipolaronic CDW.

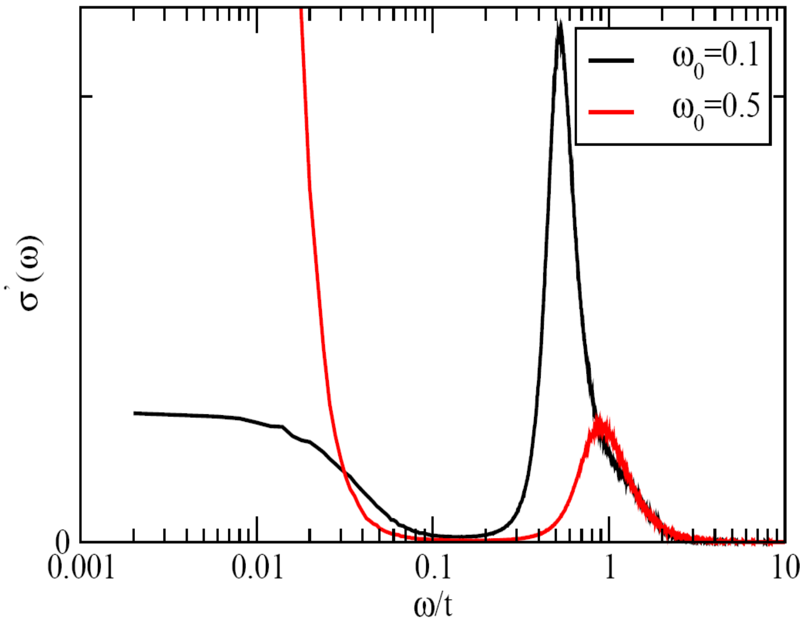
Growth of charge velocity. Mobility of bipolarons.

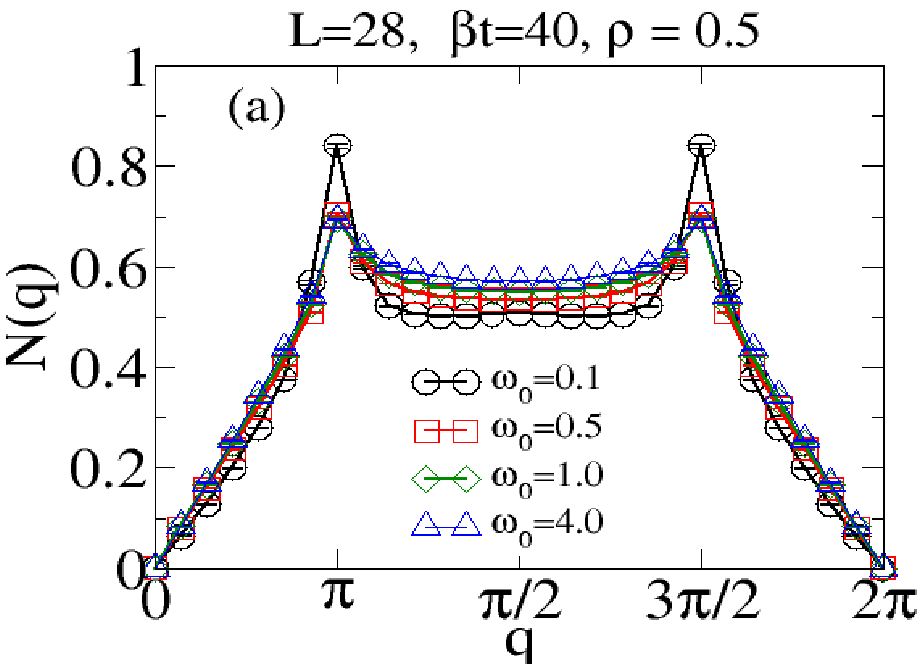
Optical Conductivity.

Continuity equation: $\sigma'(\mathbf{q},\omega) = \frac{\omega}{\mathbf{q}^2}\left(1-e^{-\beta\omega}\right) N(\mathbf{q},\omega)$

Long wavelength limit: $N(\mathbf{q},\omega) \approx N(\mathbf{q})\delta\left(v_c\mathbf{q}-\omega\right)$ with $N(\mathbf{q}) \approx \alpha\mathbf{q}$

$\rightarrow \sigma'(\omega) = \lim_{\mathbf{q}\to 0} \sigma'(\mathbf{q},\omega) \approx \alpha\, v_c \delta(\omega)$ at T=0.

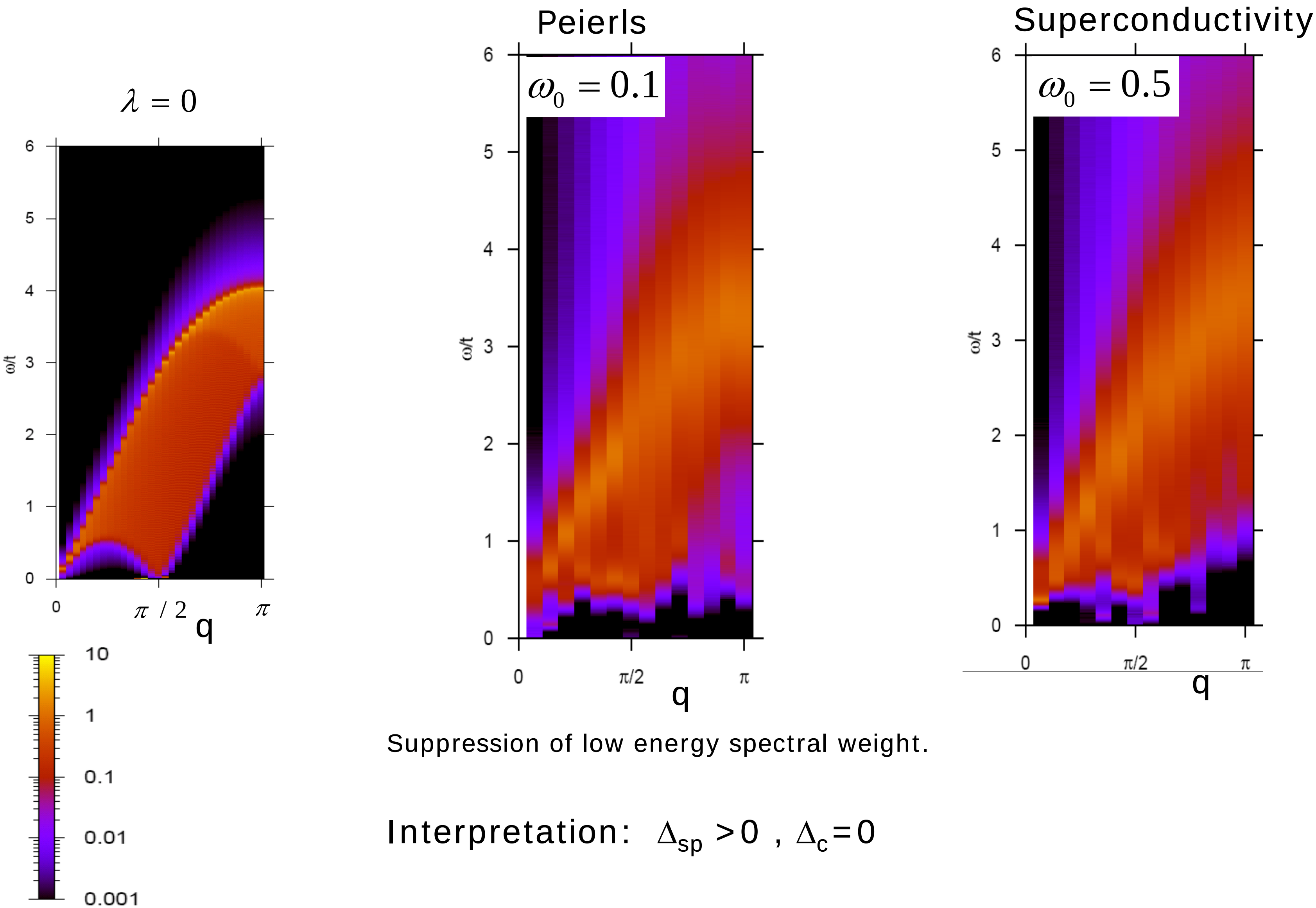




Spin dynamical structure factor. DDQMC lattice simulations. $\lambda=0.35$

$$S(q,\omega)=\frac{1}{Z}\sum_{n,m}e^{-\beta E_m}\left|\langle n|\hat{S}_z(q)|m\rangle\right|^2\delta(E_n-E_m-\omega)$$

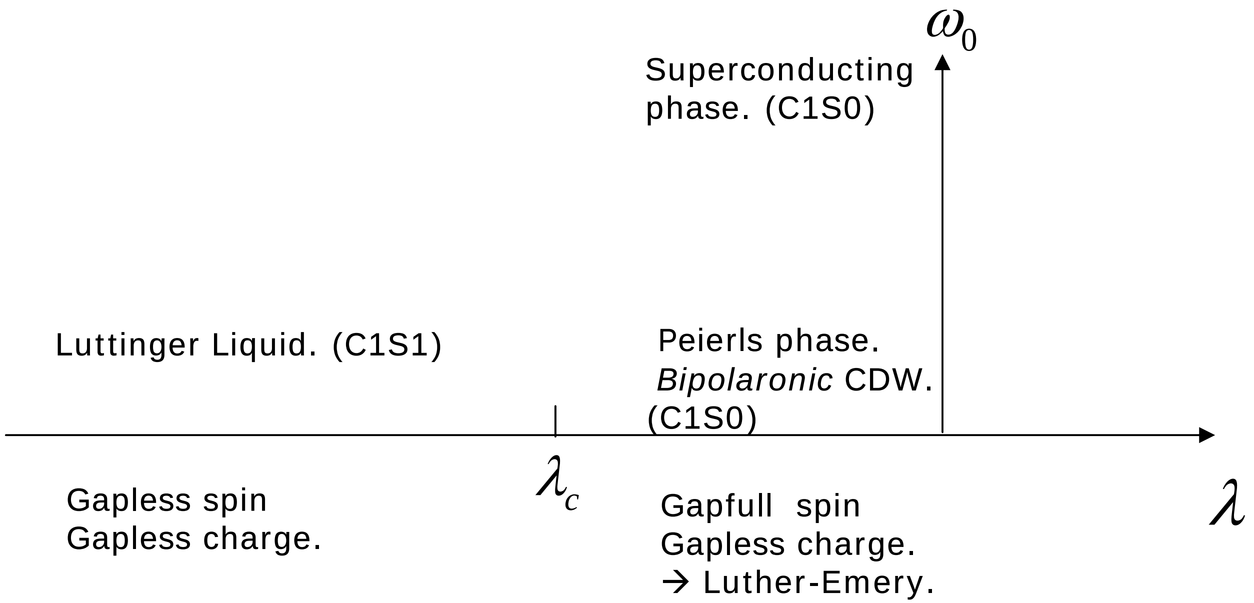
$\beta t = 40, \ \rho = 0.5$



Suppression of low energy spectral weight.

Interpretation: $\Delta_{sp} > 0$, $\Delta_c = 0$

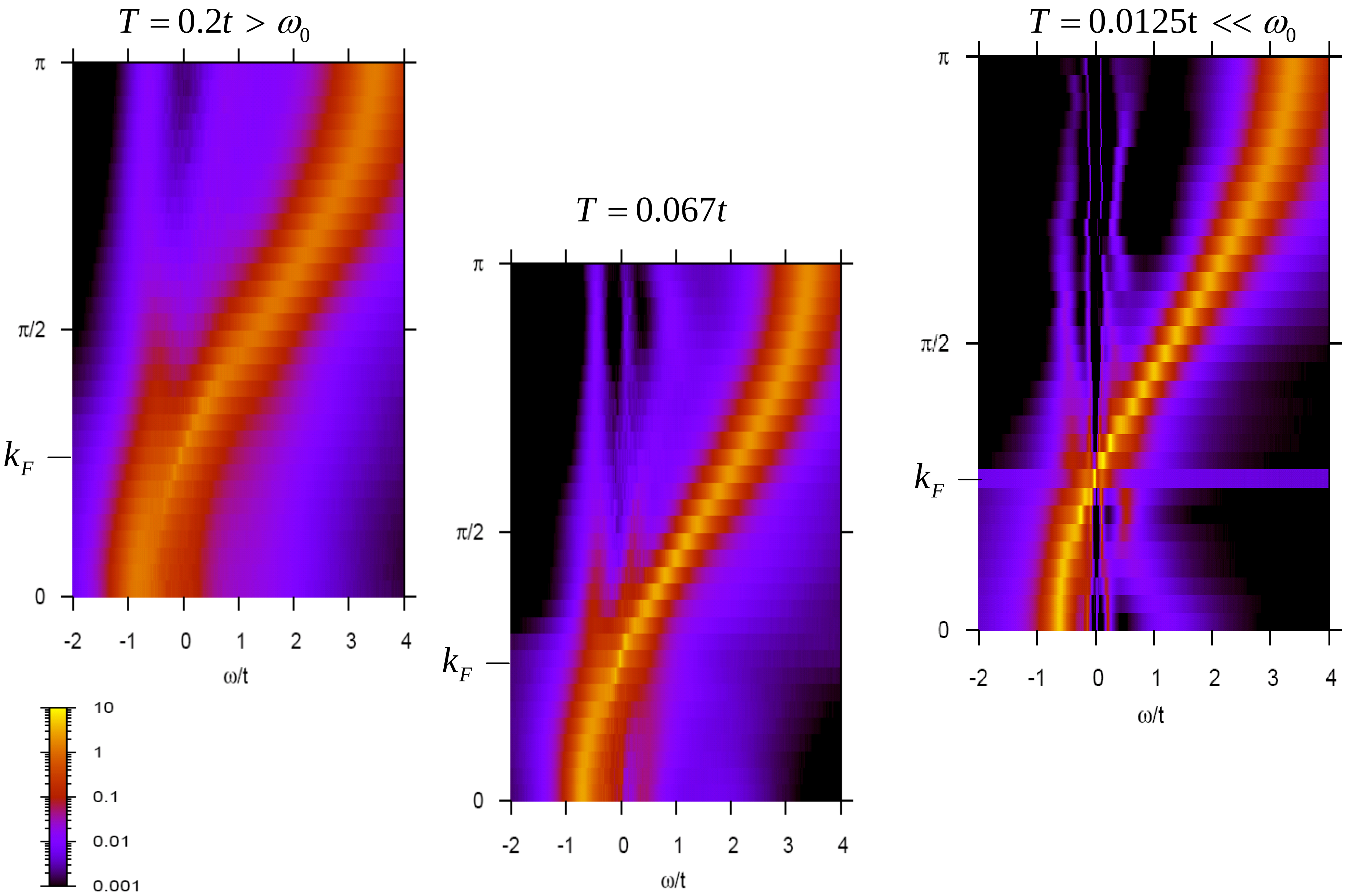
→ Two particle data is consistent with:



→ Confirmation with single particle spectral function.

b) Single particle spectral function. Lattice model. Luttinger Liquid phase. CDMFT $L_c = 8$.

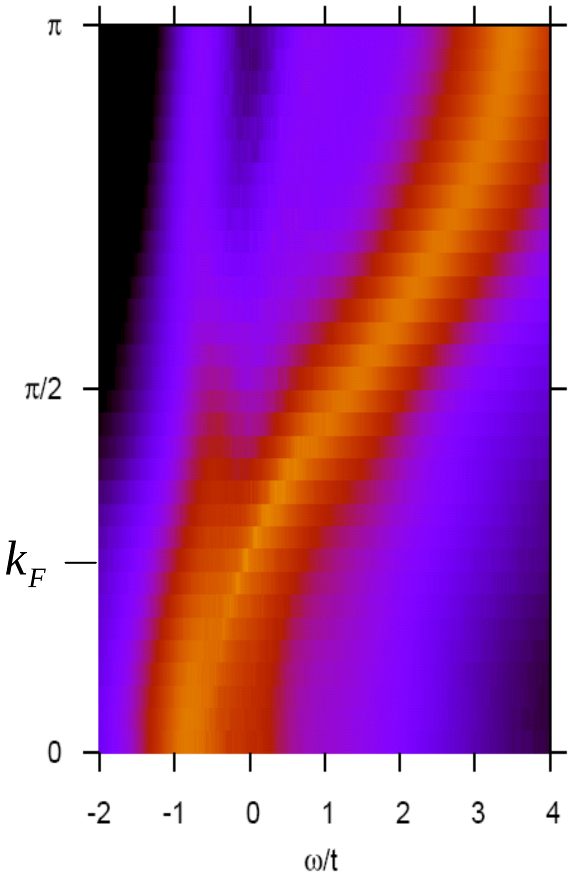
$$\lambda = 0.25, \quad \omega_0 = 0.1t, \quad \rho = 0.5$$

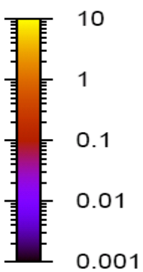


b) Single particle spectral function. Lattice model. Luttinger Liquid phase. CDMFT $L_c = 8$.

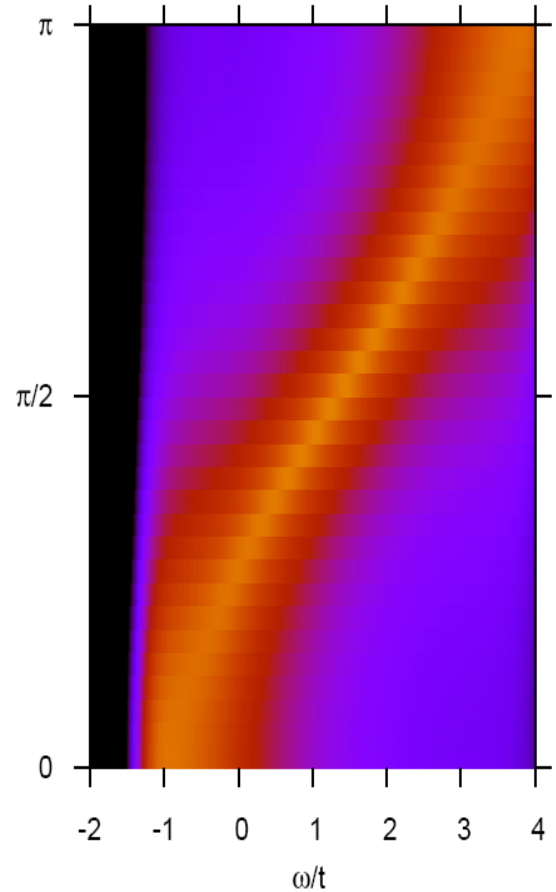
$$\lambda = 0.25, \quad \omega_0 = 0.1t, \quad \rho = 0.5$$

QMC $T = 0.2t > \omega_0$



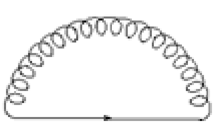


Self-consistent Born Approximation.



Engelsberg, Schrieffer Phys. Rev. 1963

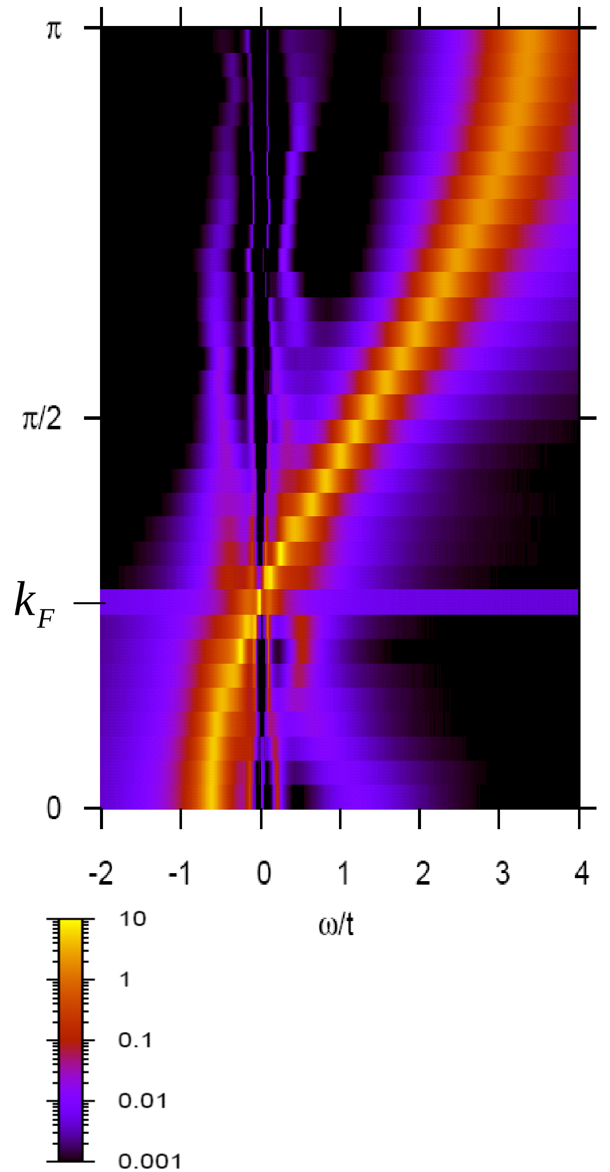
$$\Sigma(i\omega_m) =$$



b) Single particle spectral function. Lattice model. Luttinger Liquid phase. CDMFT $L_c=8$.

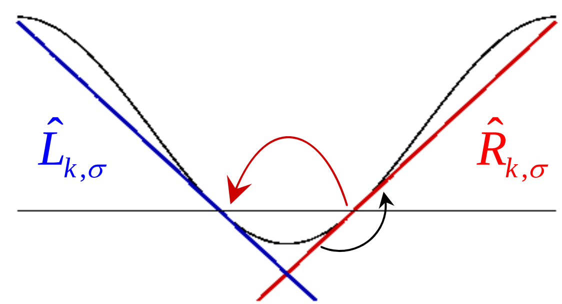
$$\lambda = 0.25,\quad \omega_0 = 0.1t,\quad \rho = 0.5$$

QMC $T = 0.0125t << \omega_0$



Luttinger Liquid approach/Bosonization.

Meden, Schönhammer, Gunnarson, PRB 94.



$$\sum_{\boldsymbol{k},\sigma} \epsilon(\boldsymbol{k}) \hat{c}^\dagger_{\boldsymbol{k},\sigma} \hat{c}_{\boldsymbol{k},\sigma} \rightarrow \sum_{\boldsymbol{k},\sigma} v_F \boldsymbol{k} \left(\hat{R}^\dagger_{\boldsymbol{k},\sigma} \hat{R}_{\boldsymbol{k},\sigma} - \hat{L}^\dagger_{\boldsymbol{k},\sigma} \hat{L}_{\boldsymbol{k},\sigma} \right)$$

Electron-Phonon interaction.

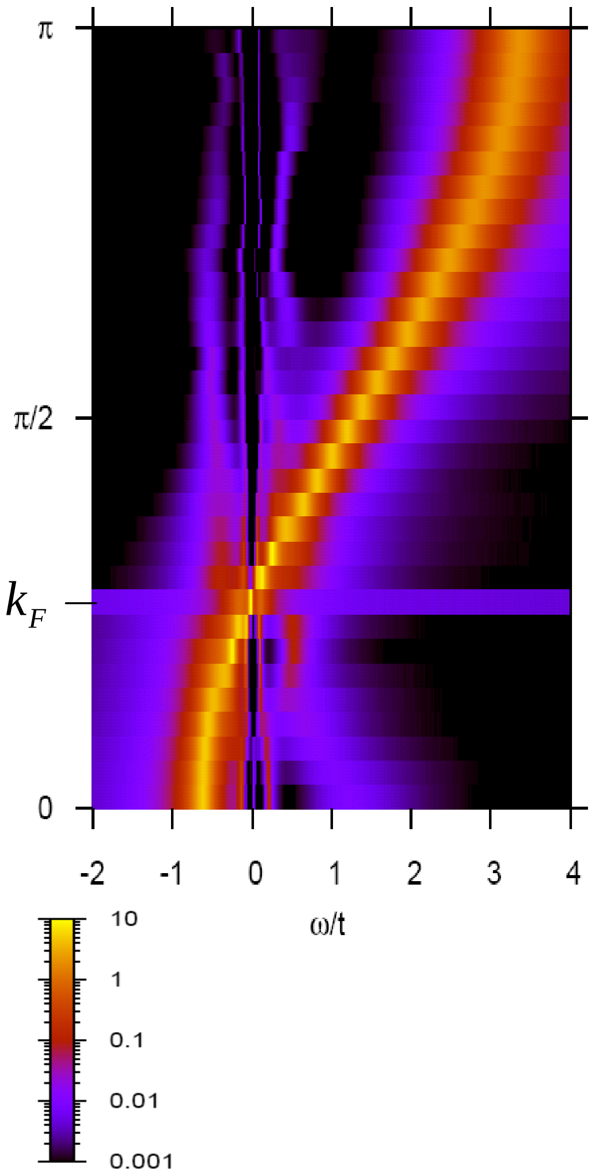
Phonon creation operator.

$$\frac{g}{\sqrt{2\omega_0 M L}} \sum_{\boldsymbol{q},\boldsymbol{k},\sigma} \Big\{ \hat{L}^\dagger_{\boldsymbol{k},\sigma} \hat{R}_{\boldsymbol{k}+\boldsymbol{q},\sigma} \left(\hat{a}^\dagger_{\boldsymbol{q}+2\boldsymbol{k}_f} + \hat{a}_{-\boldsymbol{q}-2\boldsymbol{k}_f} \right) + \hat{R}^\dagger_{\boldsymbol{k},\sigma} \hat{L}_{\boldsymbol{k}+\boldsymbol{q},\sigma} \left(\hat{a}^\dagger_{\boldsymbol{q}-2\boldsymbol{k}_f} + \hat{a}_{-\boldsymbol{q}+2\boldsymbol{k}_f} \right) + \left(\hat{L}^\dagger_{\boldsymbol{k},\sigma} \hat{L}_{\boldsymbol{k}+\boldsymbol{q},\sigma} + \hat{R}^\dagger_{\boldsymbol{k},\sigma} \hat{R}_{\boldsymbol{k}+\boldsymbol{q},\sigma} \right) \left(\hat{a}^\dagger_{\boldsymbol{q}} + \hat{a}_{-\boldsymbol{q}} \right) \Big\}. \quad (16)$$

b) Single particle spectral function. Lattice model. Luttinger Liquid phase. CDMFT $L_c = 8$.

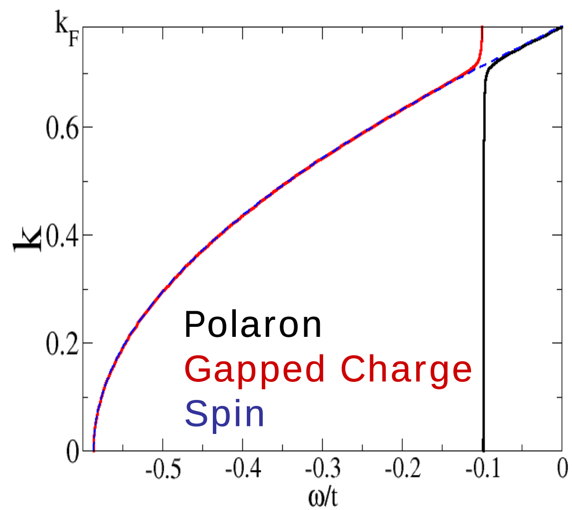
$$\lambda = 0.25, \quad \omega_0 = 0.1t, \quad \rho = 0.5$$

QMC $T = 0.0125t << \omega_0$



Luttinger Liquid approach/Bosonization.

Meden, Schönhammer , Gunnarson, PRB 94.



$$\hat{H}_{LL} = \sum_{\boldsymbol{q}} v_F |\boldsymbol{q}| \hat{\sigma}^\dagger_{\boldsymbol{q}} \hat{\sigma}_{\boldsymbol{q}} + \sum_{\boldsymbol{q}} v_F |\boldsymbol{q}| \hat{\rho}^\dagger_{\boldsymbol{q}} \hat{\rho}_{\boldsymbol{q}} + \omega_0 \sum_{\boldsymbol{q}} \hat{a}^\dagger_{\boldsymbol{q}} \hat{a}_{\boldsymbol{q}} + \sqrt{\frac{g}{2\omega_0 M \pi}} \sum_{\boldsymbol{q}} |\boldsymbol{q}| \left(\hat{\rho}^\dagger_{-\boldsymbol{q}} + \hat{\rho}_{\boldsymbol{q}} \right) \left(\hat{a}^\dagger_{\boldsymbol{q}} + \hat{a}_{-\boldsymbol{q}} \right) \quad (19)$$

$\hat{\sigma}_q$: Spin density (boson), decouples.

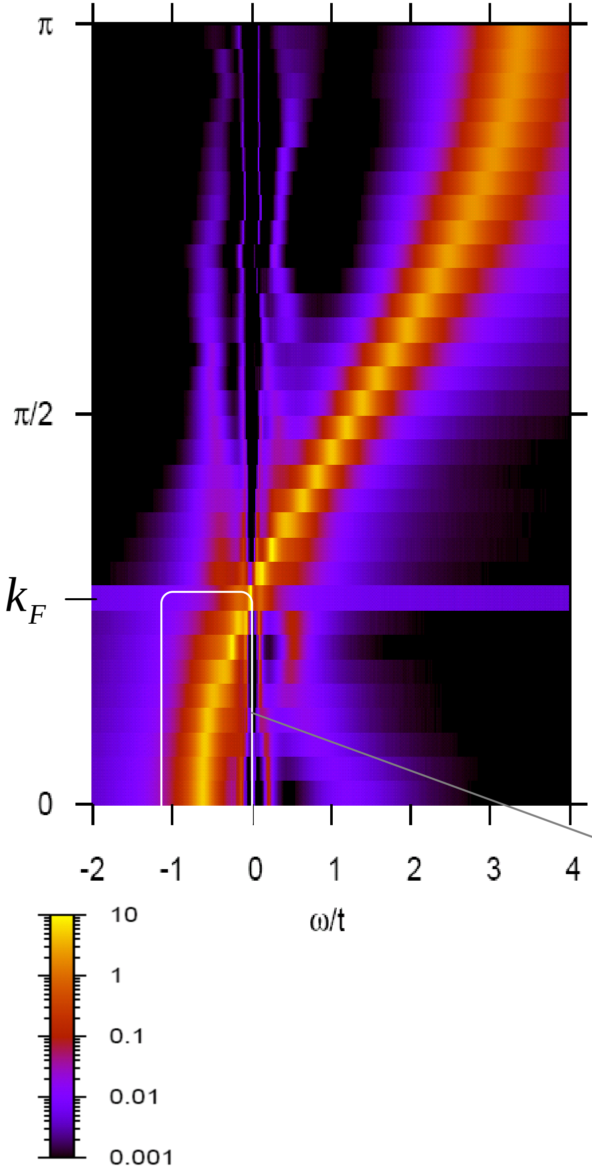
$\hat{\rho}_q$: Charge density (boson), mixes with phonon.

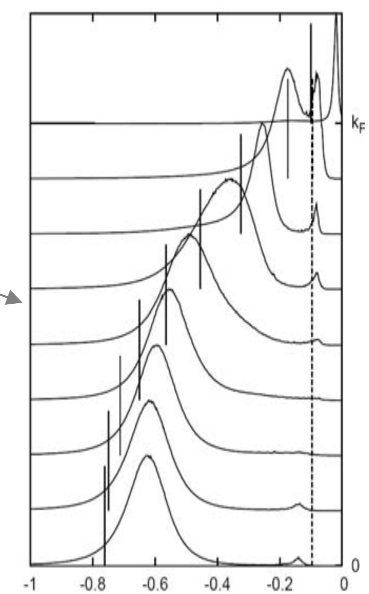
→ Bogoliubov transformation.

b) Single particle spectral function. Lattice model. Luttinger Liquid phase. CDMFT $L_c = 8$.

$$\lambda = 0.25, \quad \omega_0 = 0.1t, \quad \rho = 0.5$$

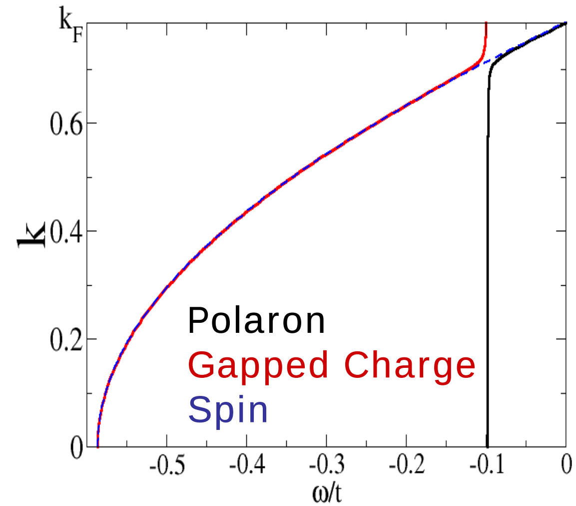
QMC $T = 0.0125t << \omega_0$





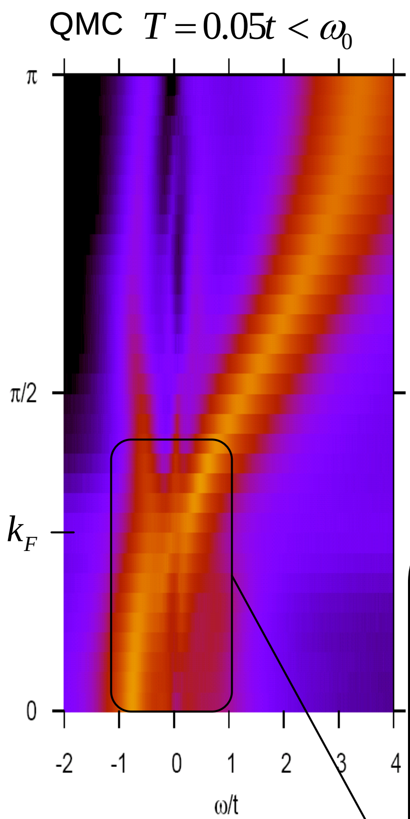
Luttinger Liquid approach/Bosonization.

Meden, Schönhammer , Gunnarson, PRB 94.



b) Single particle spectral function. Peierls phase insulating phase. CDMFT $L_c = 12$.

$$\lambda = 0.35, \quad \omega_0 = 0.1t, \quad \rho = 0.5$$

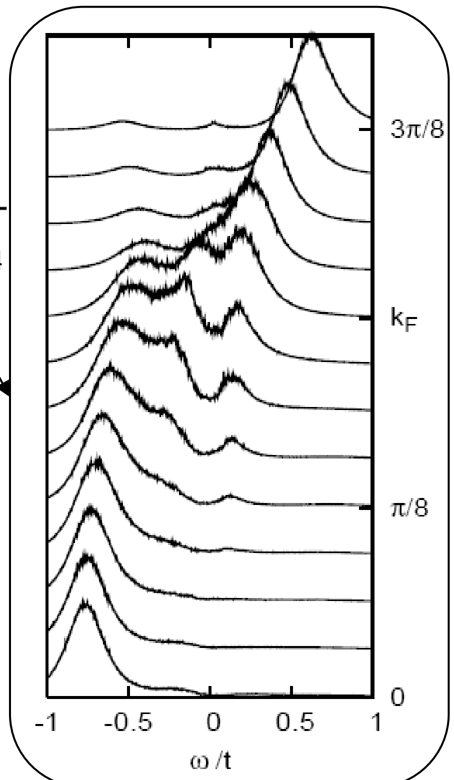


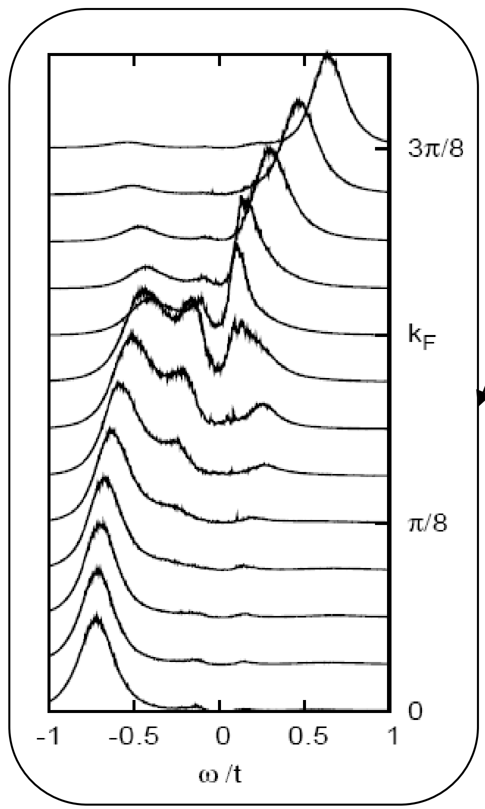
Interpretation:

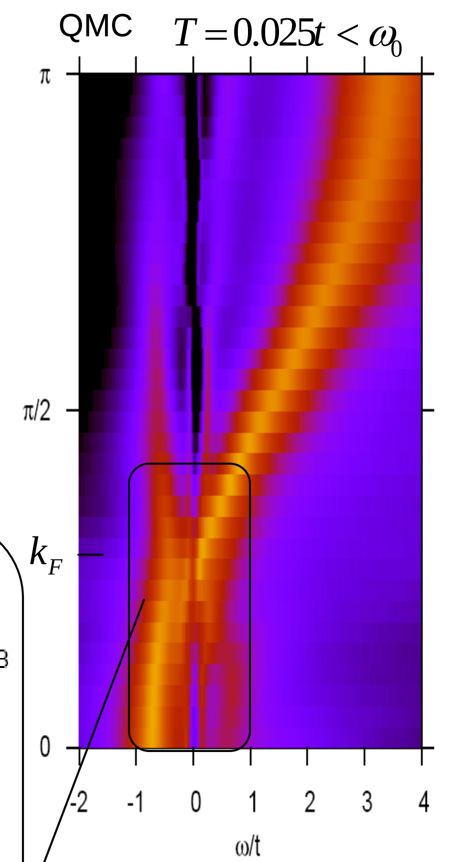
Breaking of a bipolaron.

Energy cost is the spin gap:
$\Delta_{sp} \sim 0.2t \sim 2\Delta_{qp}$

Consistent with Luther-Emery liquid.





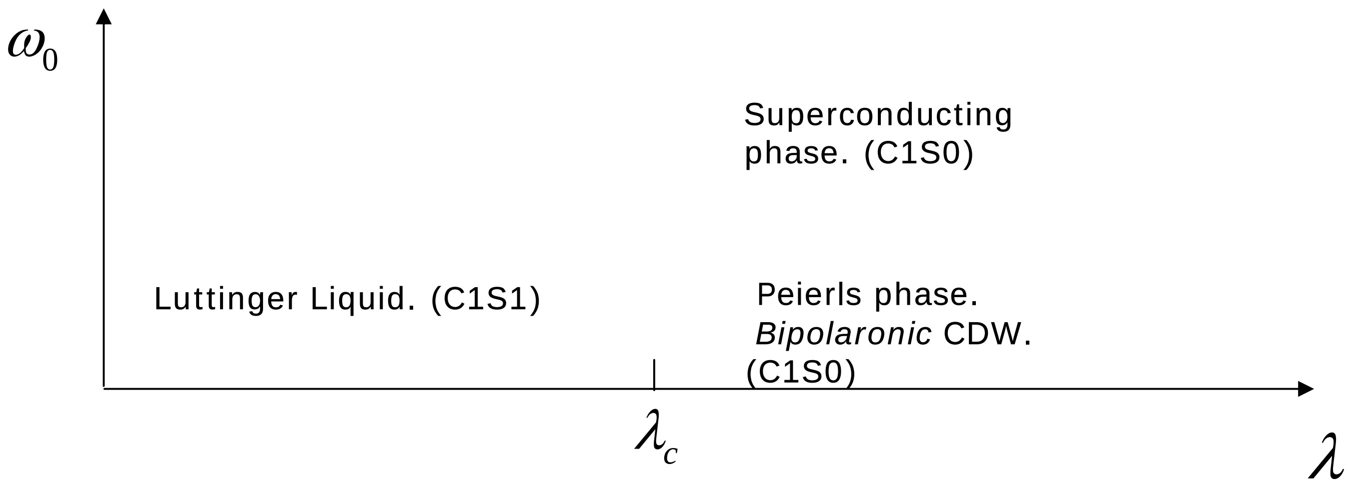


Summary.

Weak-coupling CT-QMC.

- Simple and flexible method. Perfectly suited for cluster methods (DCA, CDMFT)
- Allows to acces "large" clusters.
- Generalization to projective schemes (M. Feldbacher, K Held, FFA PRL 2004). ✓
- Generalization to include phonons, retarded interactions. ✓

¼ Filled Holstein model .



Charge, spin and single particle spectral functions, and temperature dependence thereof. ✓

→ SSH phonons.

→ Phonons + Electronic correlation (Heavy fermions, TTF-TCNQ).