Weak-Coupling CT-QMC: projective schemes and applications to retarded interactions.

F.F. Assaad (IPAM January 26-30, 2009)

Outline

- Weak coupling CT-QMC (Rubtsov et al. PRB 05).
- Projective schemes.
- 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)

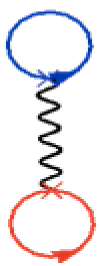
I. The method. Anderson Model (Rubtsov et. al PRB (05))

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

Dyson. Expansion around U=0.

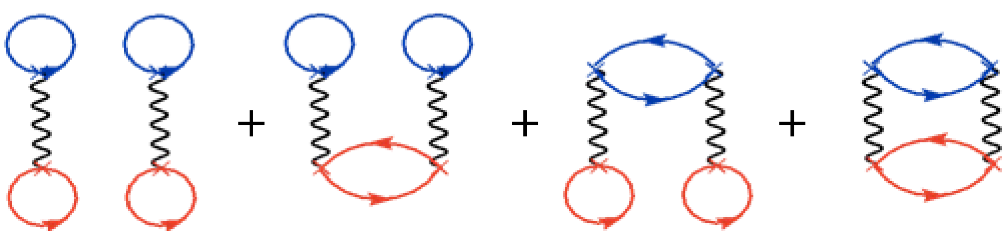
$$\frac{\mathrm{Tr}\left[e^{-\beta H}\right]}{\mathrm{Tr}\left[e^{-\beta H_0}\right]} = \sum_n \int_0^\beta d\tau_1 \cdots \int_0^{\tau_{n-1}} d\tau_n\, (-U)^n \left\langle n_\uparrow(\tau_1) n_\downarrow(\tau_1) \cdots n_\uparrow(\tau_n) n_\downarrow(\tau_n) \right\rangle_0$$

Wick

n=1  $G_0^{\uparrow}$ U $G_0^{\downarrow}$

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

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

n=2 

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

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

Weight / Sign.

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

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

→ 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.

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

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

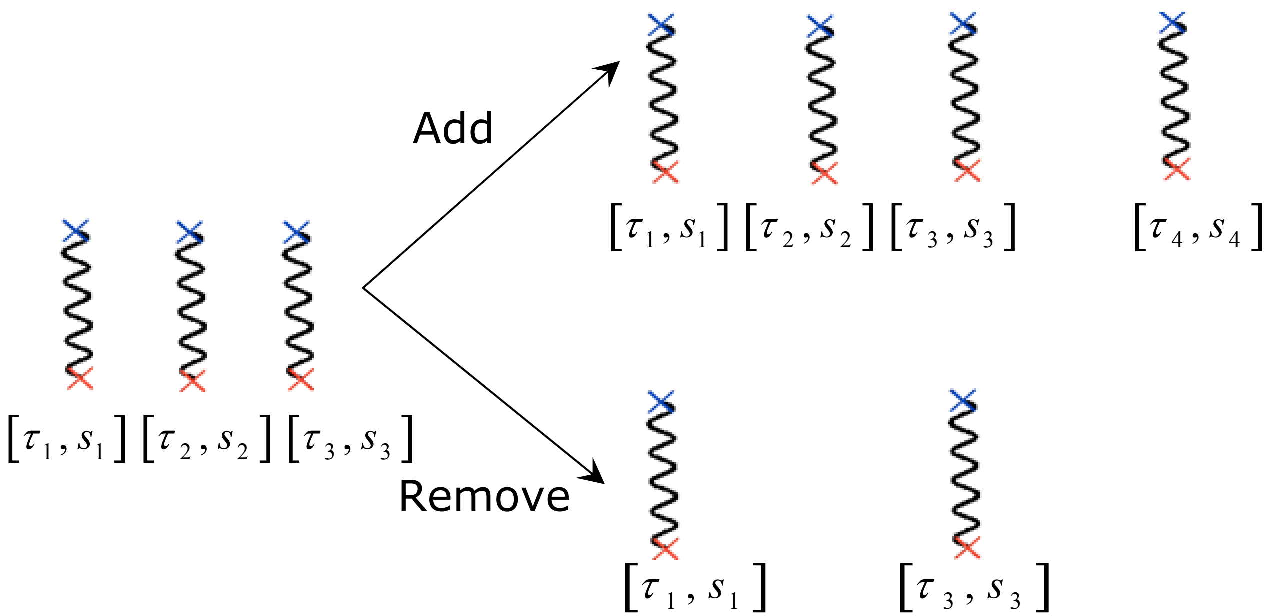
- $$H_U = U\left(n_\uparrow{}^d - [1/2 - \delta]\right)\left(n_\downarrow{}^d - [1/2 + \delta]\right) + \underbrace{U\delta(n_\uparrow{}^d - n_\downarrow{}^d)}_{\text{Absorb in } H_0}$$

- 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.

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

Wick theorem applies for each configuration C of vertices.

Direct calculation of Matsubara Green functions.

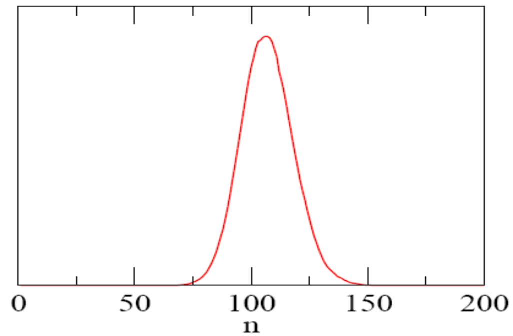
$$G^\sigma{}_C(i\omega_m) = G^\sigma{}_0(i\omega_m) - G^\sigma{}_0(i\omega_m)\sum_{\alpha,\beta=1}^n e^{-i\omega_m\tau_\alpha}\left(M^\sigma{}_n{}^{-1}\right)_{\alpha\beta} G^\sigma{}_0(\tau_\beta,0)$$

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

Average Expansion parameter.

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

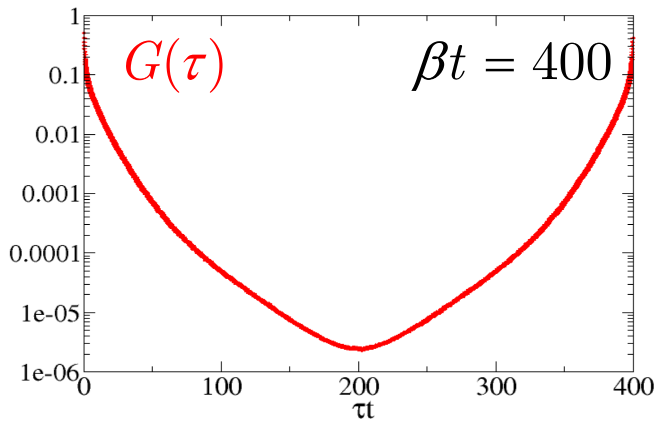
- CPU time scales as $\langle n \rangle^3$ → same scaling as Hirsch-Fye.
- <n> is minimal at particle-hole symmetric point, $\delta = 0$



Histogram of expansion parameter.

Examples.

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

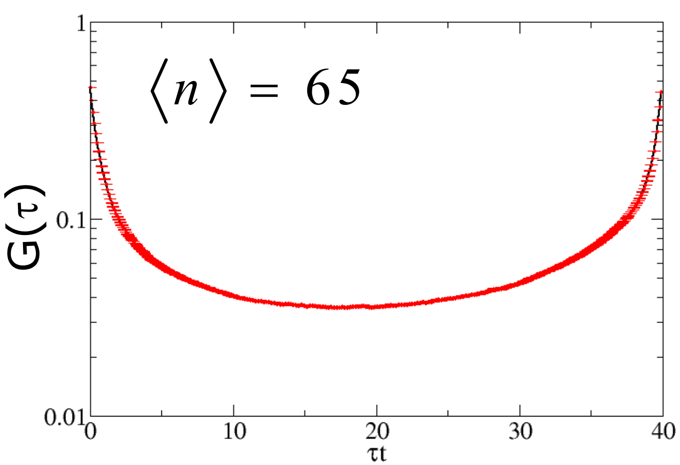


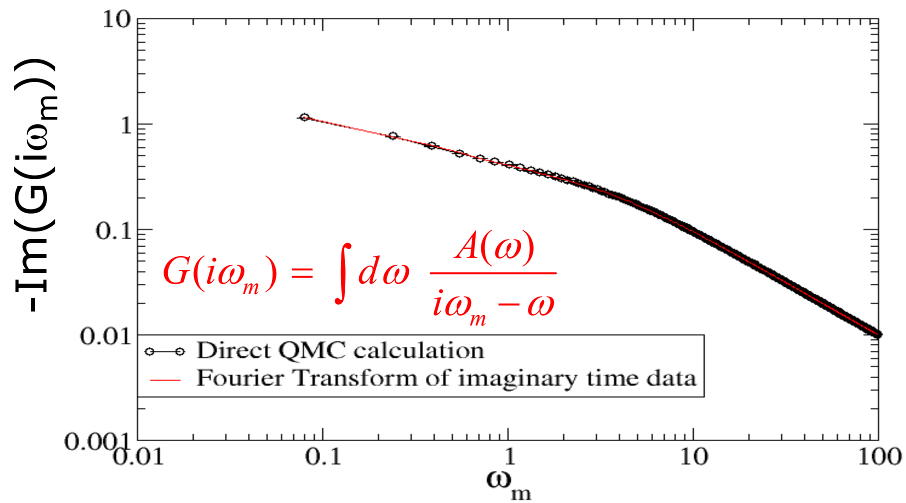
$\langle n \rangle = 270$

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.

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II) Projective Schemes

Ground state	Finite temperature
$\langle O \rangle_0 = \lim_{\theta \to \infty} \frac{\langle \Psi_T \vert e^{-\frac{\theta}{2}H} O \, e^{-\frac{\theta}{2}H} \vert \Psi_T \rangle}{\langle \Psi_T \vert e^{-\theta H} \vert \Psi_T \rangle}$	$\langle O \rangle = \frac{\mathrm{Tr}\, e^{-\beta H} O}{\mathrm{Tr}\, e^{-\beta H}}$
No thermal fluctuations	Thermal fluctuations

Formulation.

$$\frac{\langle \psi_T \vert e^{-\theta H} \vert \psi_T \rangle}{\langle \psi_T \vert \psi_T \rangle} = \sum_n \int_0^{\theta} d\tau_1 \sum_{s_1} \cdots \int_0^{\tau_{n-1}} d\tau_n \sum_{s_n} \left(-\frac{U}{2} \right)^n \det\left[M_n \left(\tau_1, s_1 \cdots, \tau_n, s_n \right) \right]$$

Replace $G_0^{\sigma}(\tau_2,\tau_1) = \langle T \hat{d}_{\sigma}^{+}(\tau_2) \hat{d}_{\sigma}(\tau_1) \rangle$ by $\frac{\langle \psi_T \vert T \hat{d}_{\sigma}^{+}(\tau_2) \hat{d}_{\sigma}(\tau_1) \vert \psi_T \rangle}{\langle \psi_T \vert \psi_T \rangle}$ in determinant.

Note: $\vert \psi_T \rangle$ has to be a Slater determinant !

PQMC+DMFT

DMFT: self-consistency cycle.

$$\Sigma(i\omega) \Rightarrow \boxed{\text{Dyson}} \Rightarrow G(i\omega) = \int d\varepsilon \frac{N(\varepsilon)}{i\omega - \varepsilon + \mu - \Sigma(i\omega)}$$

$$\Uparrow \qquad\qquad \Downarrow \mathcal{G}_0^{-1}(i\omega) = G^{-1}(i\omega) - \Sigma(i\omega)$$

$$G(\tau) \Leftarrow \boxed{\text{PQMC}} \Leftarrow \mathcal{G}_0(\tau)$$

Question:

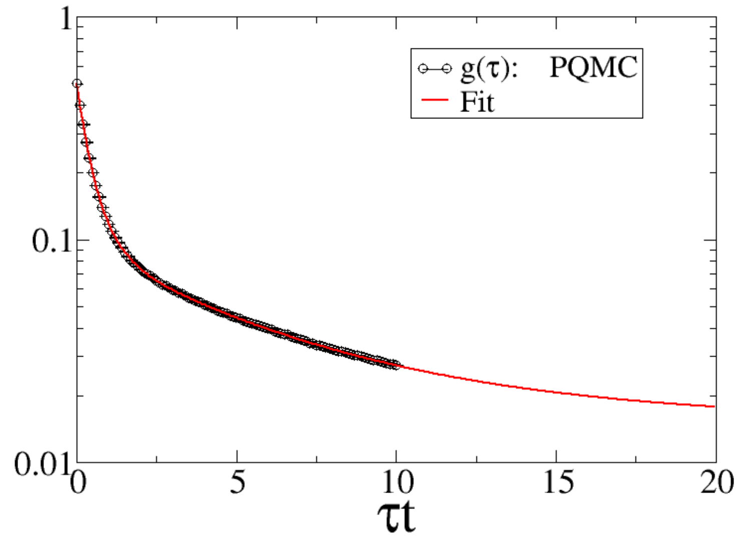
$$G(\tau) \quad \text{for} \quad \tau \in [-\theta_M, \theta_M], \quad \rightarrow \quad G(i\omega_m) = \int_{-\infty}^{\infty} d\tau \; e^{i\omega_m \tau} G(\tau) \quad ?$$

MaxEnt.

$$G(\tau) = \int d\omega \;\; K(\tau,\omega) A(\omega)$$

$$G(i\omega_m) = \int d\omega \; \frac{A(\omega)}{i\omega_m - \omega}$$

→ MaxEnt as a fitting procedure.



Example: Mott transition.

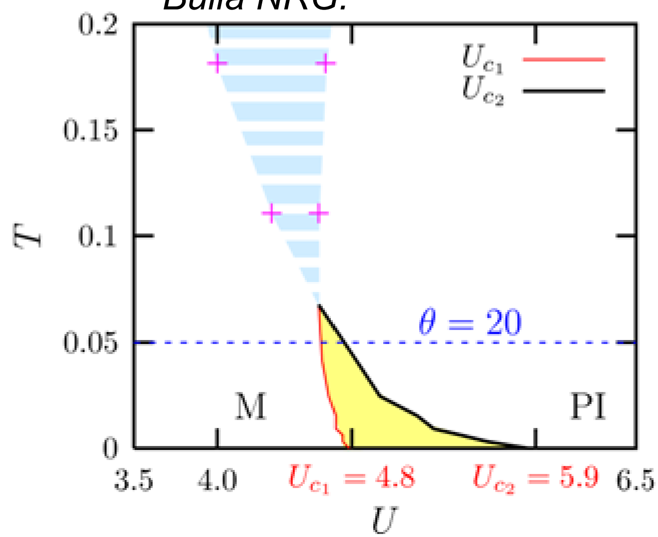
Hamiltonian:

$$\hat{H} = -t \sum_{\langle i,j \rangle} \hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + U \sum_{i} \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow}$$

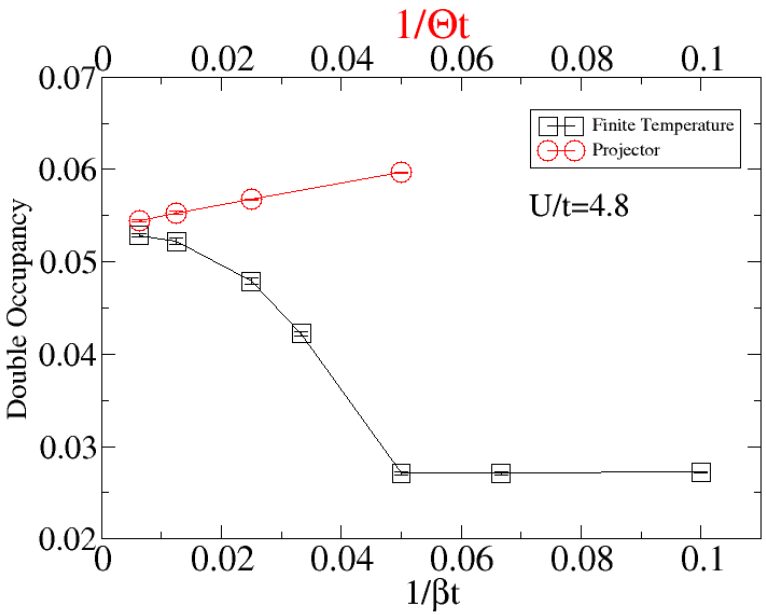
Bethe-DOS: bandwidth W=4

Phase diagram:

Bulla NRG:



PQMC vs. QMC:



Simulations at $\theta t \approx 20-30$ give good estimate of ground state properties.

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III) 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.

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

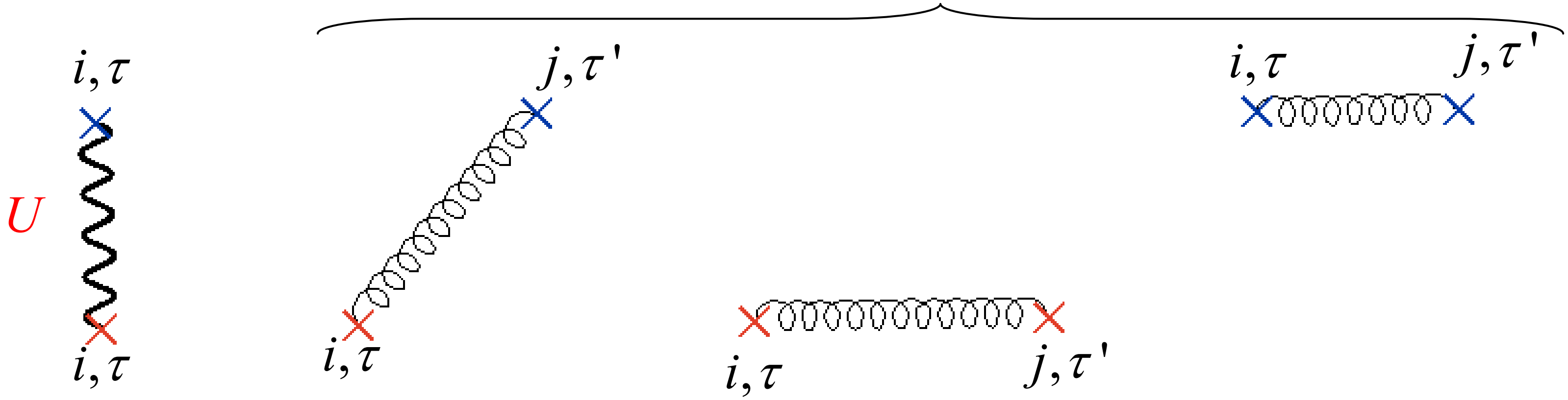
$$Z = \int \left[dc^+ dc \right] \exp\left[-S_0 - U\int_0^\beta d\tau \; n_{i\uparrow}(\tau) n_{i\downarrow}(\tau) \; + \int_0^\beta d\tau \int_0^\beta d\tau' \sum_{i,j} [n_i(\tau)-1] D^0(i-j,\tau-\tau')[n_j(\tau')-1] \right]$$

DDQMC. Expand both in Hubbard and retarded phonon interaction.

Vertices:

Hubbard.

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



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One-dimensional quarter filled Holstein model.

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

¼ Filled Holstein model @ ω_0=0.1t

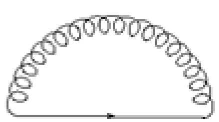
Luttinger Liquid.

Peierls phase.
Bipolaronic CDW.

λ_c — λ

Gapless spin
Gapless charge.

Gapfull spin
Gapless charge.
→ Luther-Emery.

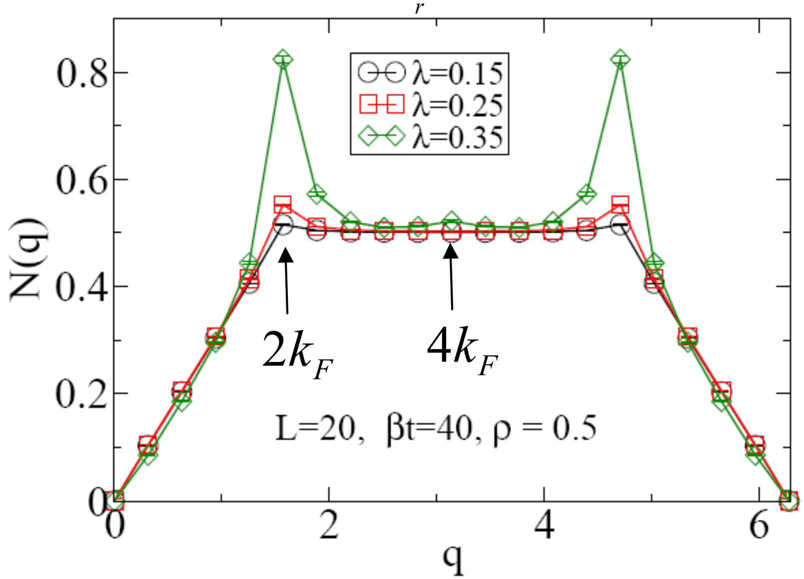
$\Sigma(i\omega_m) =$  Flat band width W → $\frac{m^*}{m} = 1 + \lambda, \quad \lambda = \frac{g^2}{2k}\frac{2}{W}$

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. Lattice simulations. ω_0=0.1t

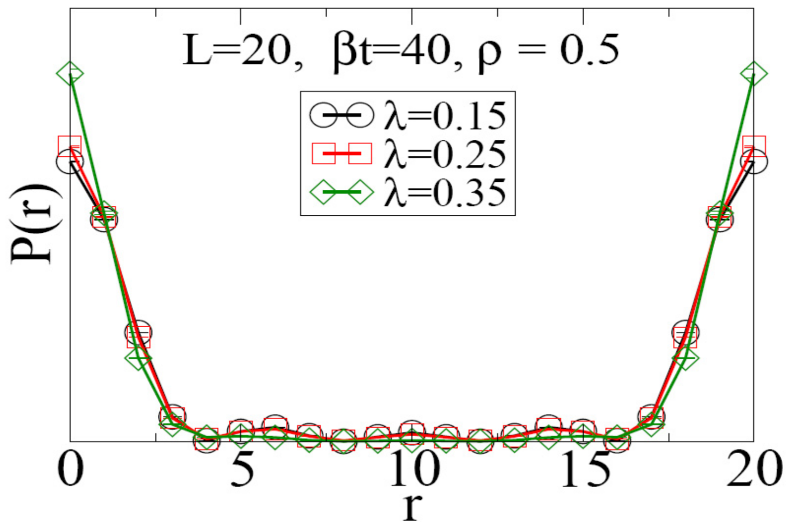
Charge $N(q) = \sum_r e^{iqr} \langle \hat{n}(r)\hat{n}(0) \rangle$



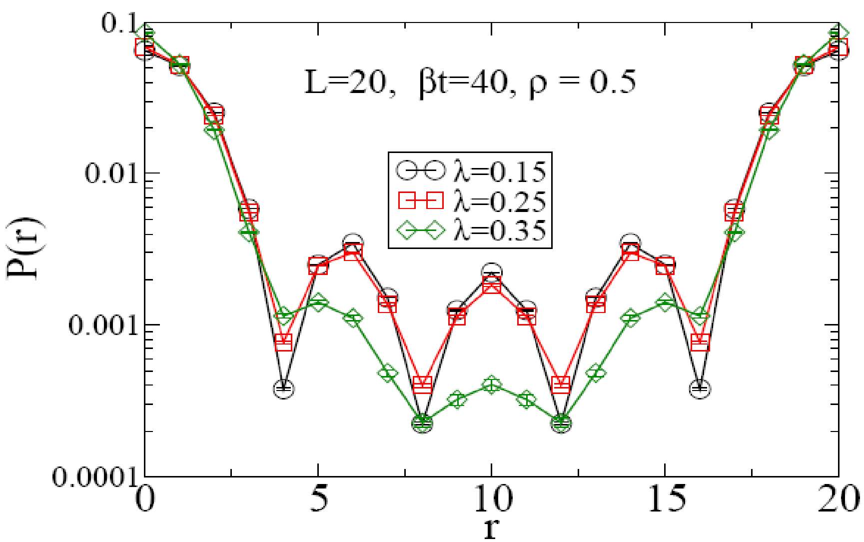
Dominant $2k_F$ charge correlations, at $\lambda \sim 0.35$

Static properties. Lattice simulations. ω_0=0.1t

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



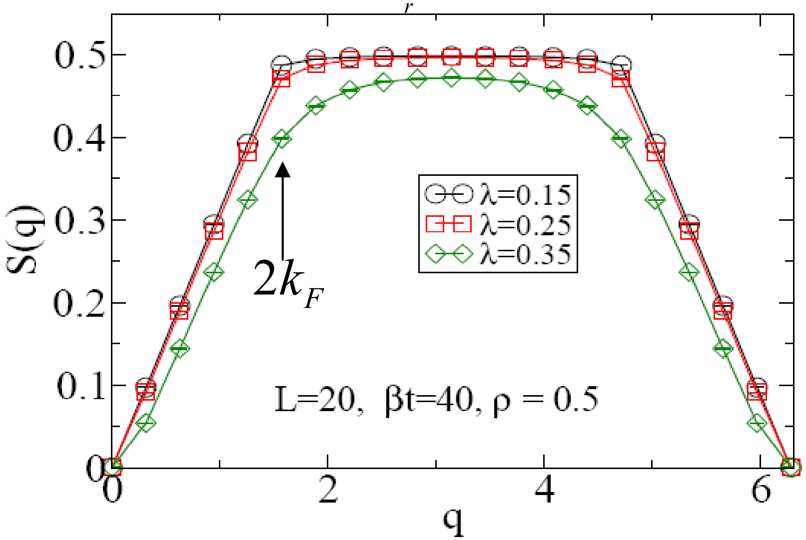
Short ranged pairing correlations grow → Two electrons with opposite spin share the same potential well (Bipolarons).



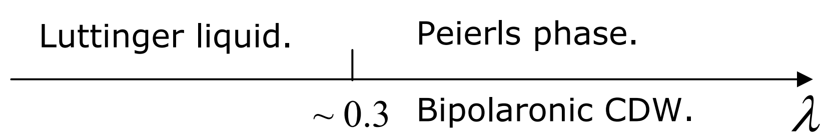
Long range pairing correlations drop → Bipolarons tend to localize.

Static properties. Lattice simulations. ω_0=0.1t

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



Pairing suppresses spin response.

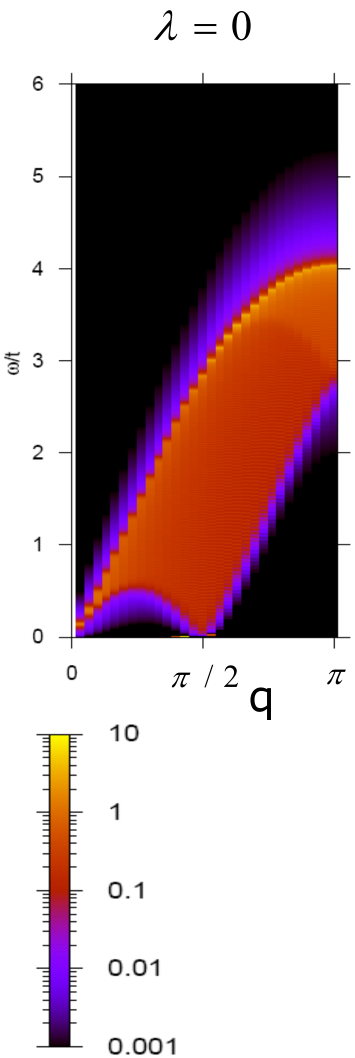


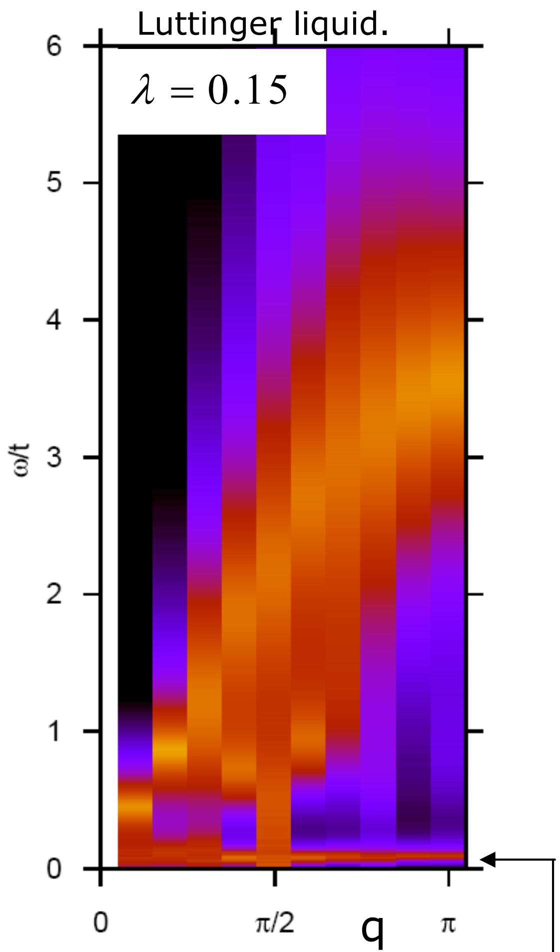
Insulator or metal?

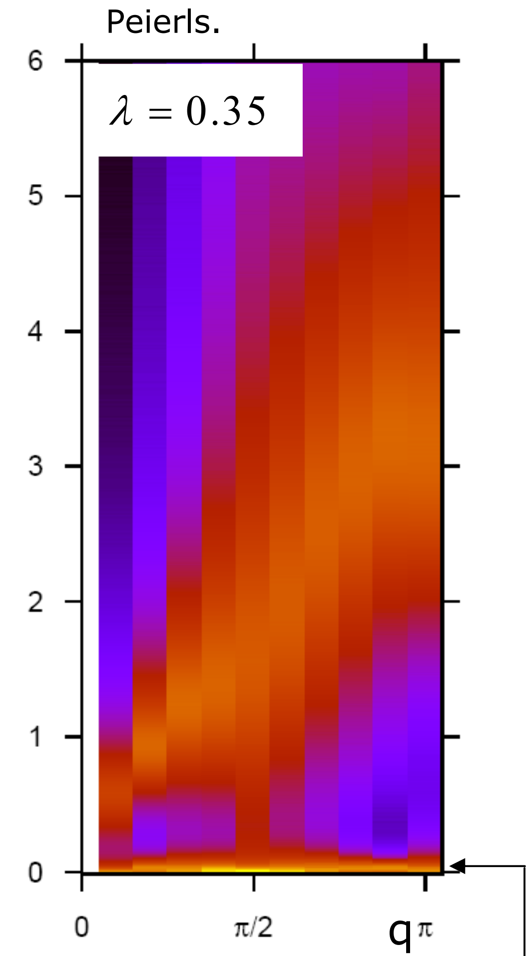
Charge dynamical structure factor. Lattice simulations. $\omega_0=0.1t$

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

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







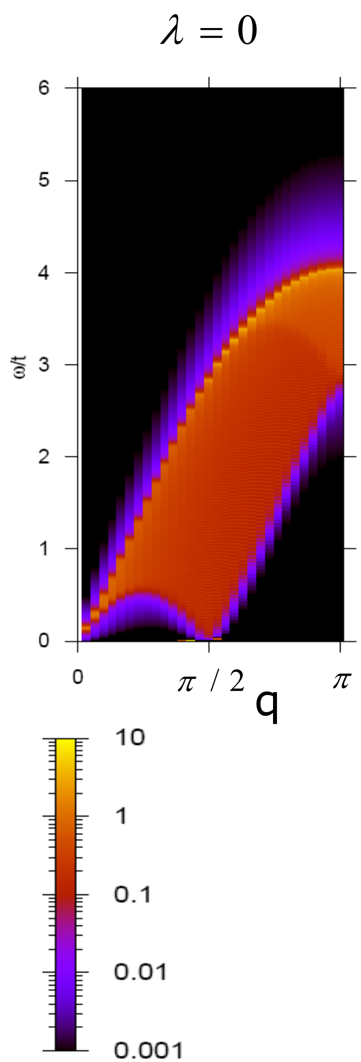
Charge couples to phonon.
→ Phonon modes are apparent in charge response.

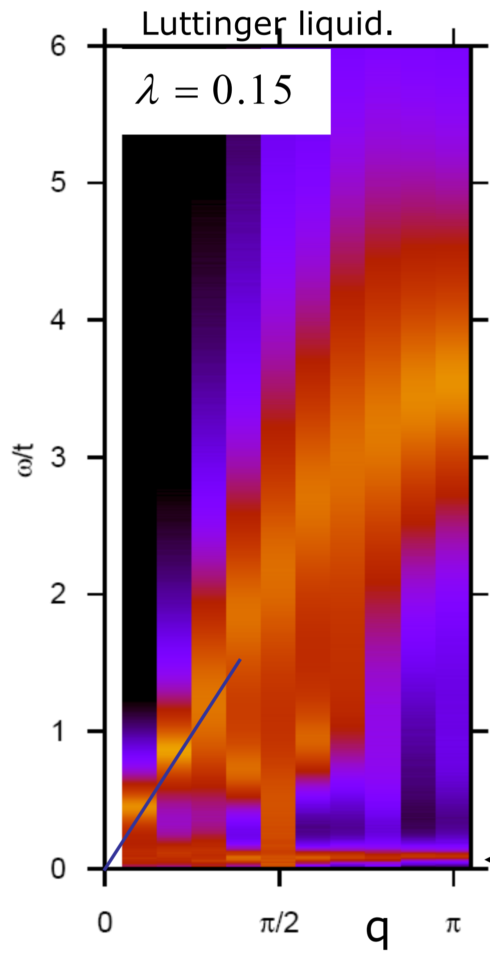
Piling up of spectral weight at $2k_f$. Slow dynamics of the CDW.

Charge dynamical structure factor. Lattice simulations. $\omega_0=0.1t$

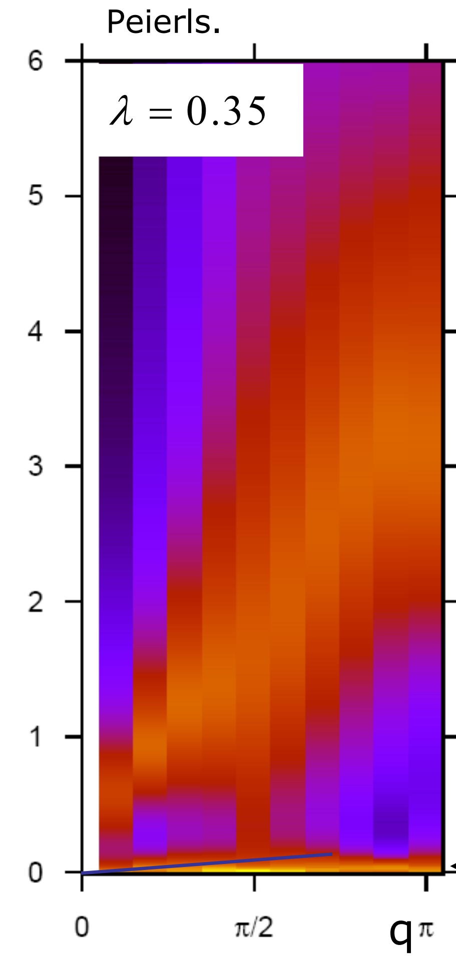
$$N(q,\omega)=\frac{1}{Z}\sum_{n,m} e^{-\beta E_m}\left|\langle n|\hat{n}\ (q)|m\rangle\right|^2 \delta(E_n-E_m-\omega)$$

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





Charge velocity?



Charge couples to phonon.
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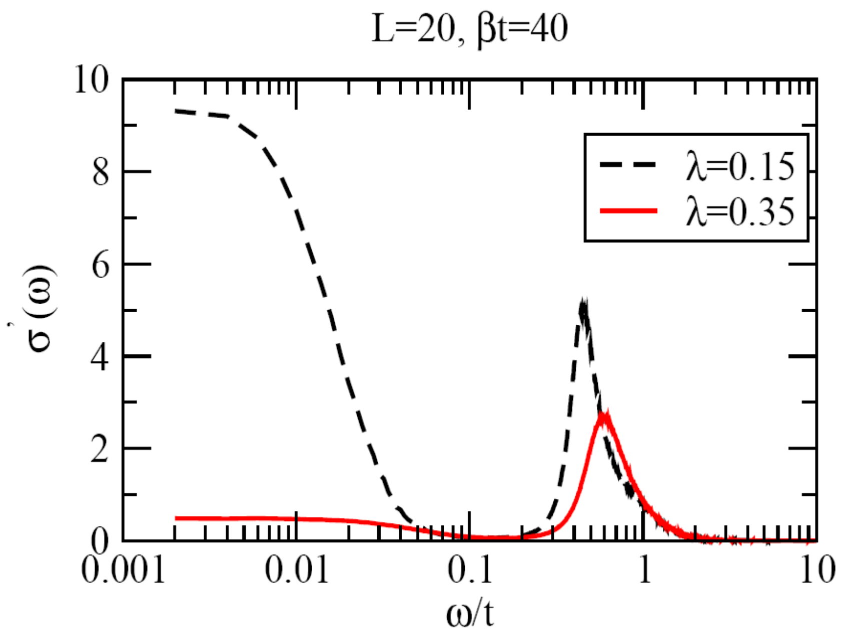
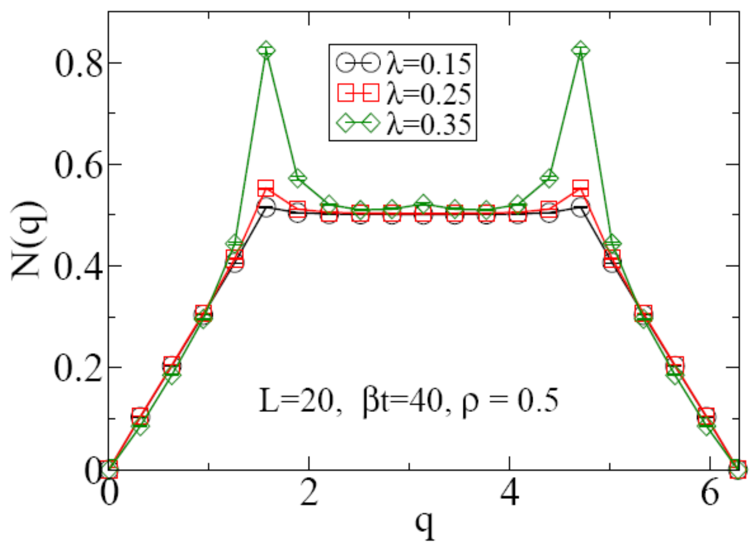
Optical Conductivity.

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 $N(\mathbf{q}) \approx \alpha\mathbf{q}$

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



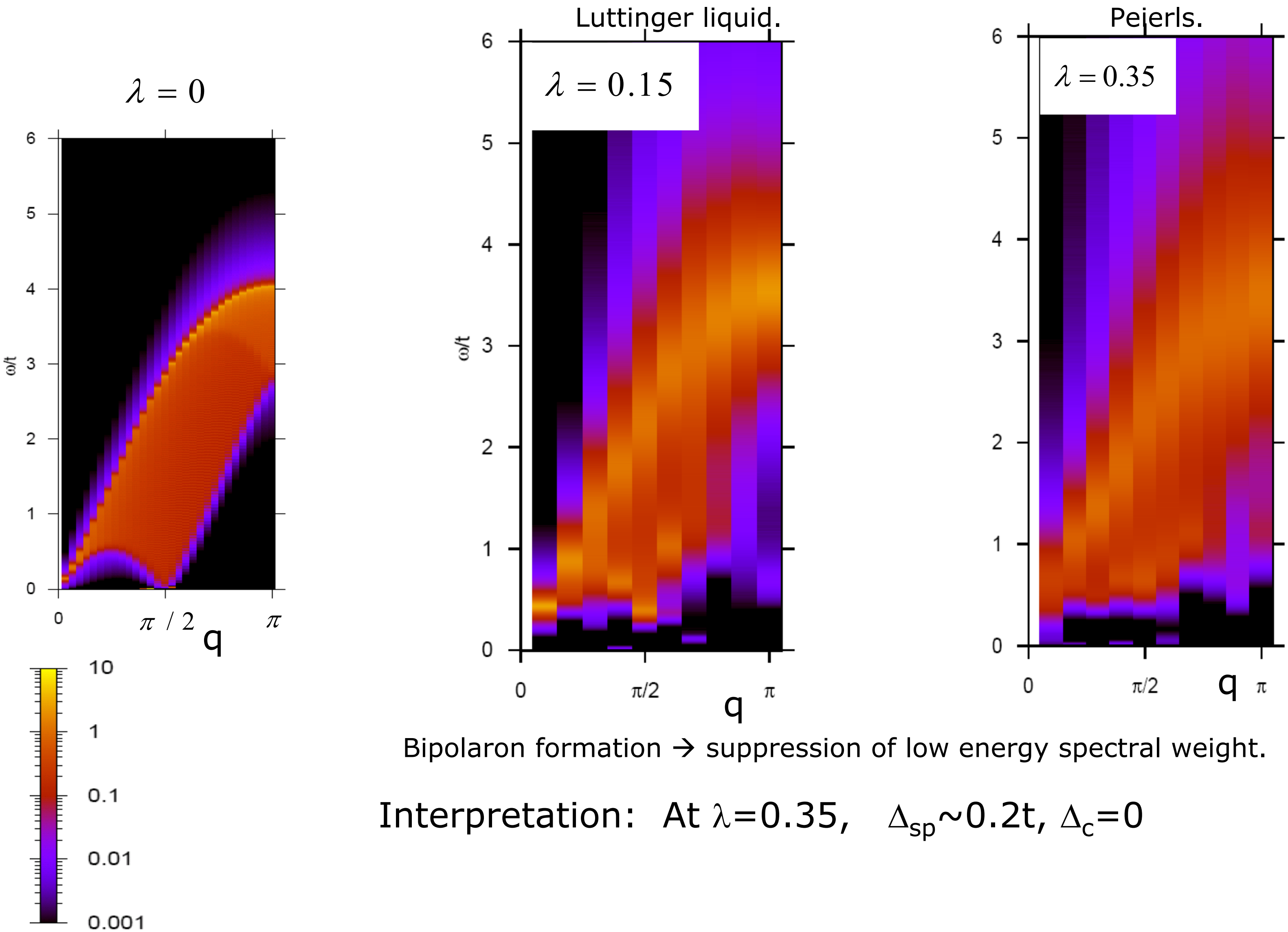


→ λ=0.35 is a metallic state!

Spin dynamical structure factor. DDQMC lattice simulations. $\omega_0=0.1t$

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

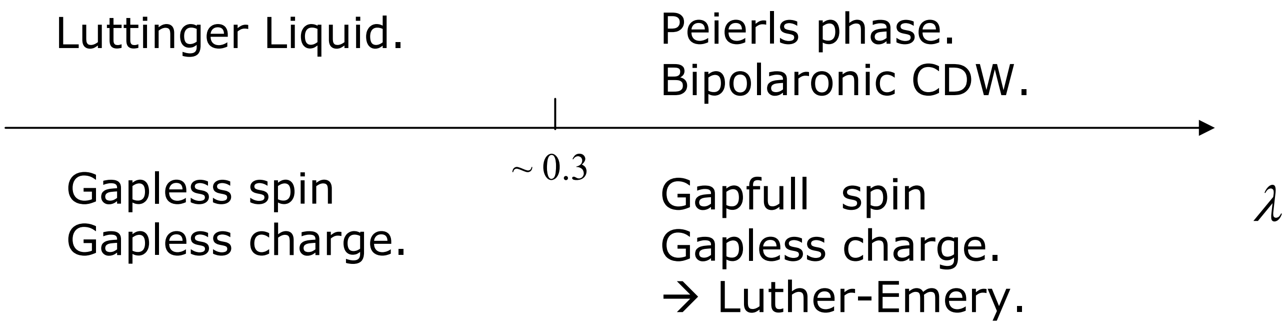
$\beta t=40,\ \rho=0.5$



Bipolaron formation → suppression of low energy spectral weight.

Interpretation: At $\lambda=0.35$, $\Delta_{sp}\sim 0.2t$, $\Delta_c=0$

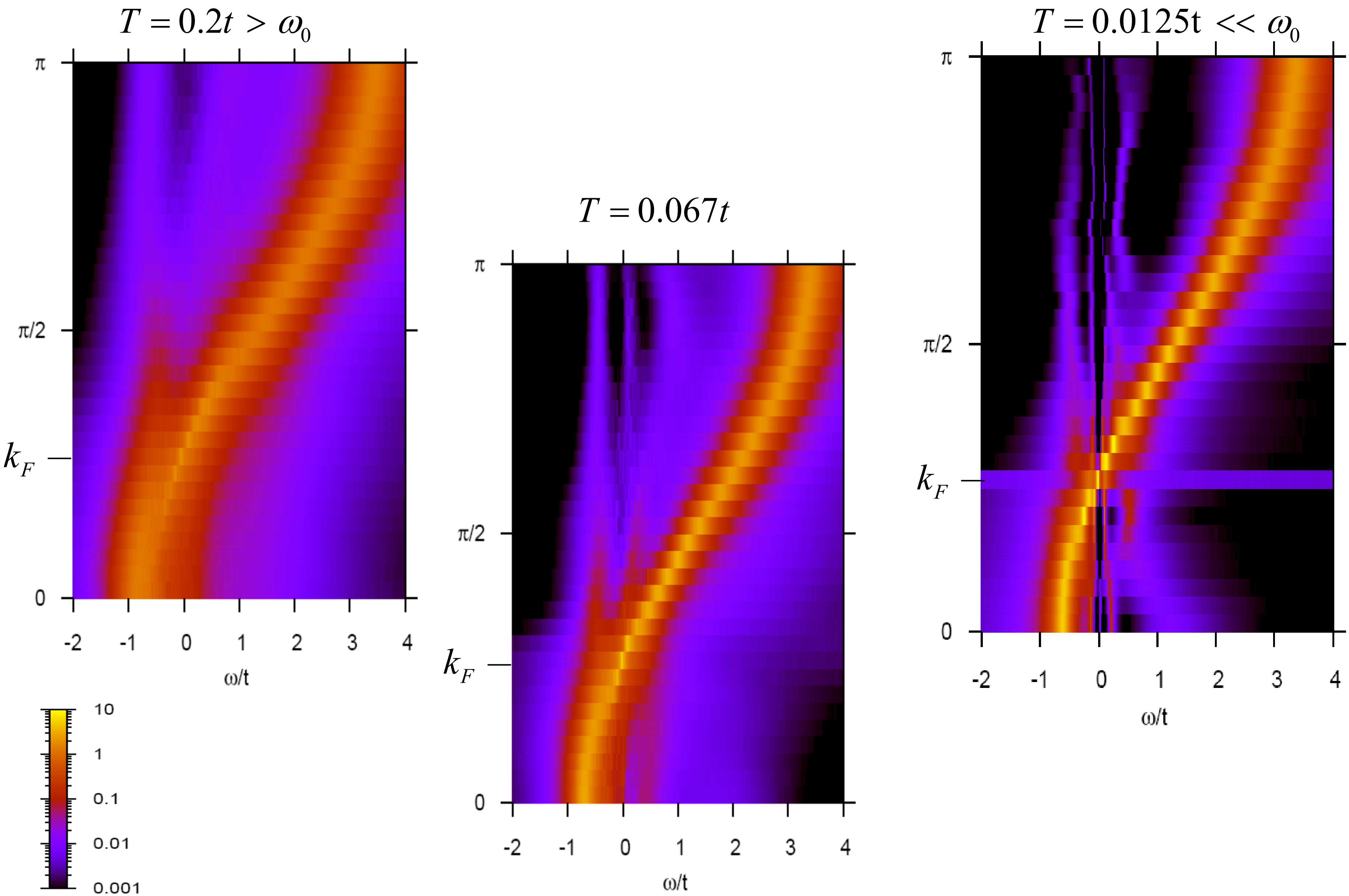
→ Two particle data is consistent with:



→ Confirmation with single particle spectral function.

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

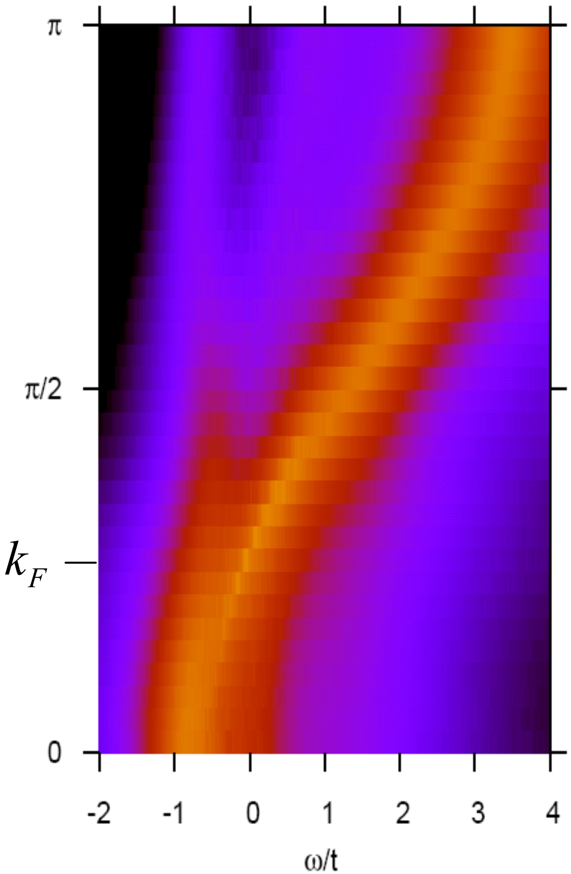
$\lambda = 0.25, \quad \omega_0 = 0.1t, \quad \rho = 0.5$

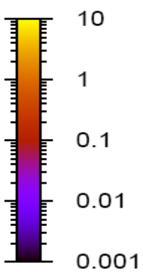


b) Single particle spectral function. Lattice model. Luttinger Liquid phase. CDMFT L_c=8.

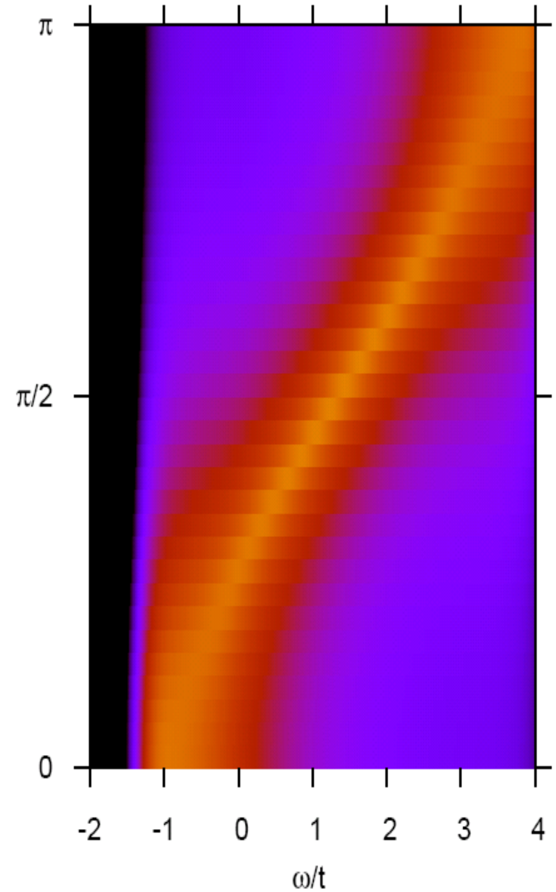
$$\lambda = 0.25,\quad \omega_0 = 0.1t,\quad \rho = 0.5$$

QMC $T = 0.2t > \omega_0$

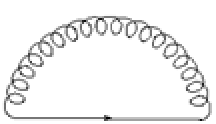




Self-consistent Born Approximation.



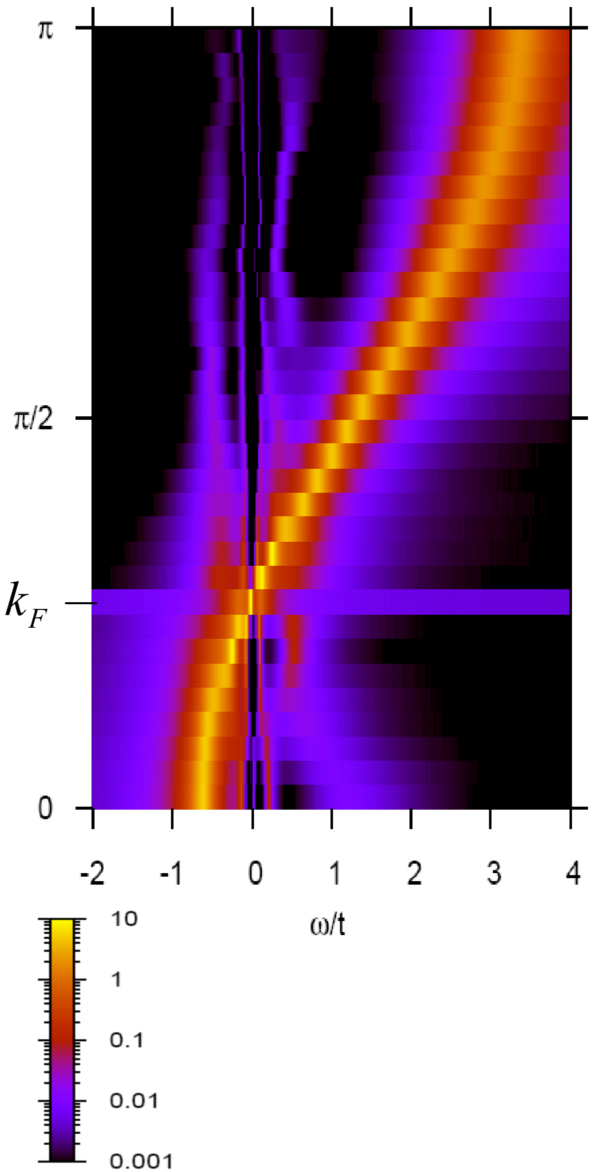
Engelsberg, Schrieffer Phys. Rev. 1963

$\Sigma(i\omega_m) =$ 

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

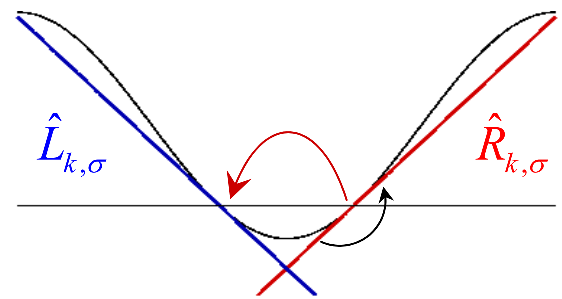
$$\lambda = 0.25, \quad \omega_0 = 0.1t, \quad \rho = 0.5$$

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.

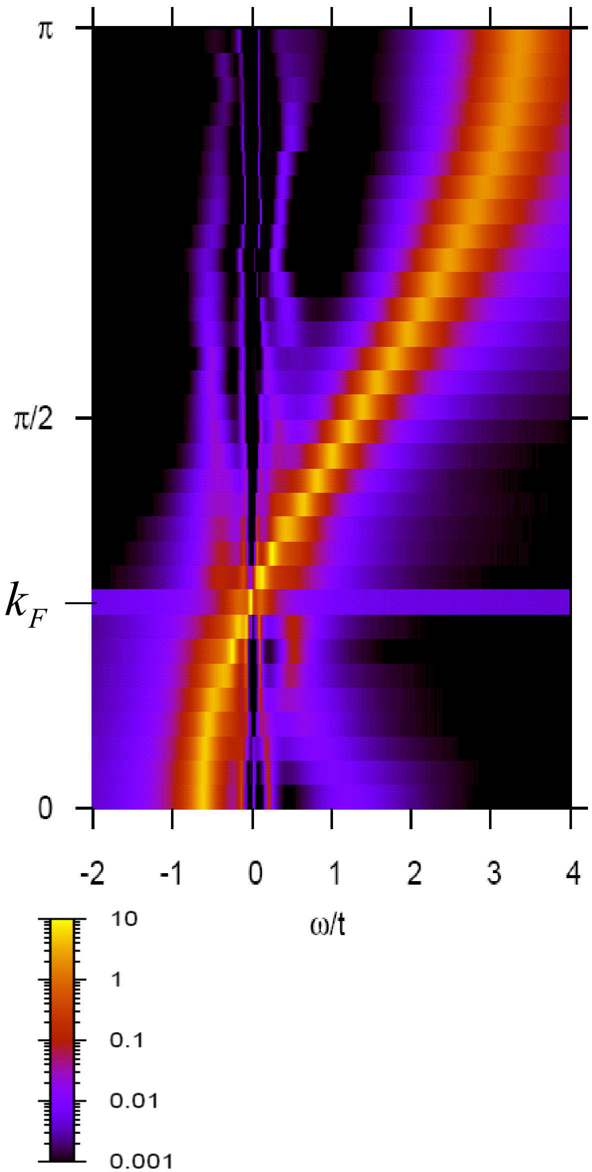
Phonon creation operator.

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

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

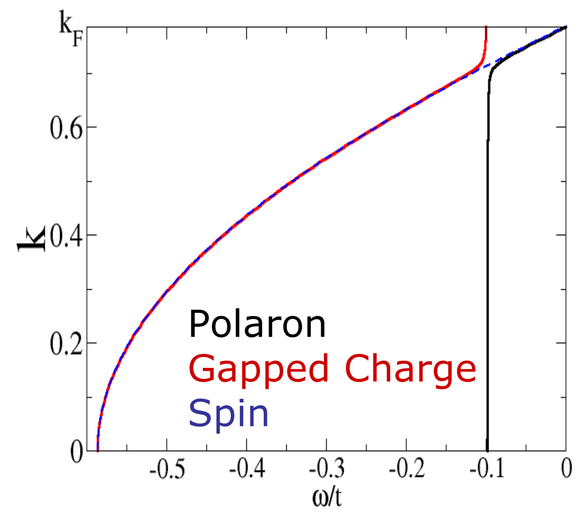
$$\lambda = 0.25, \quad \omega_0 = 0.1t, \quad \rho = 0.5$$

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.

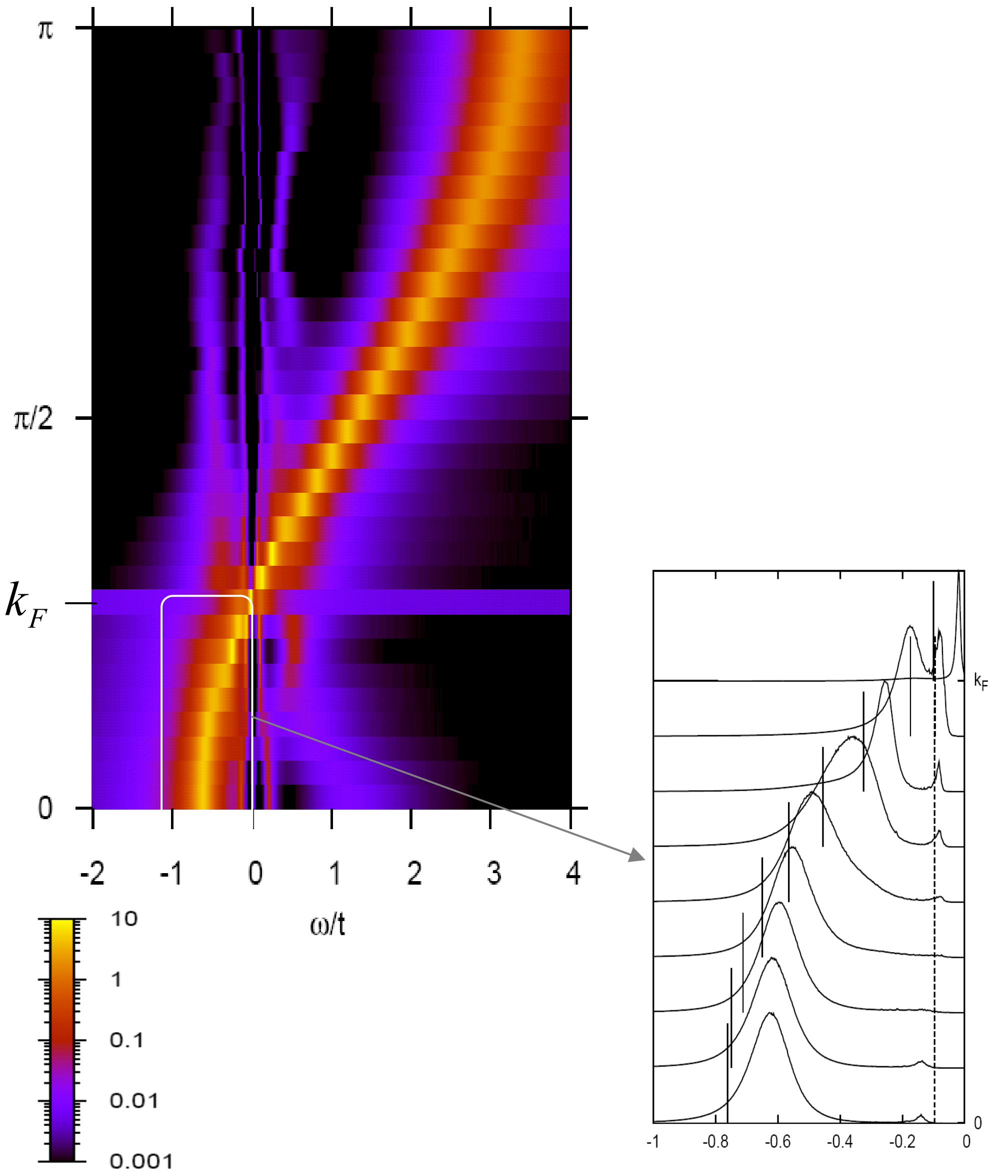
$\hat{\rho}_q$: Charge density (boson), mixes with phonon.

→ Bogoliubov transformation.

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

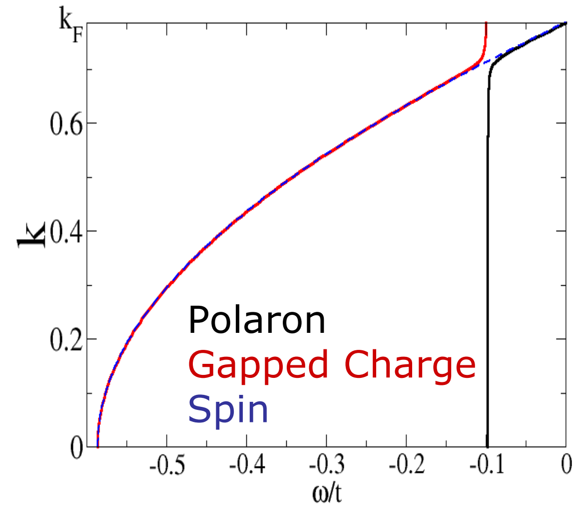
$$\lambda = 0.25, \quad \omega_0 = 0.1t, \quad \rho = 0.5$$

QMC $T = 0.0125t << \omega_0$



Luttinger Liquid approach/Bosonization.

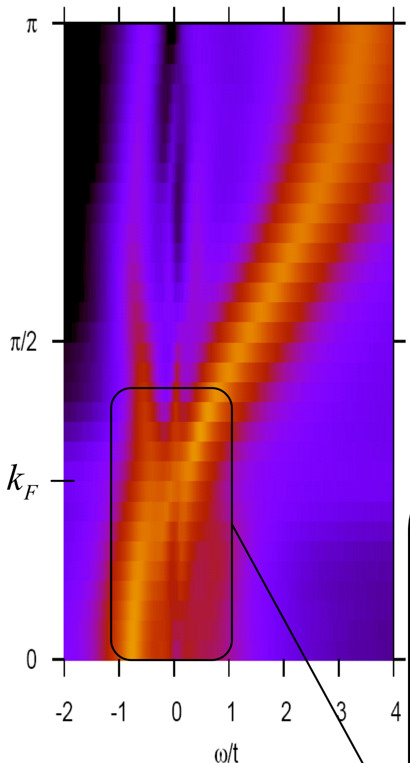
Meden, Schönhammer , Gunnarson, PRB 94.

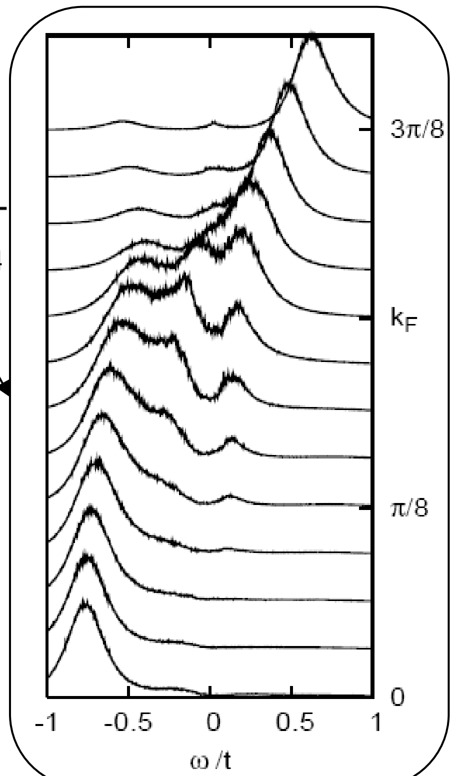


b) Single particle spectral function. Peierls phase insulating phase. CDMFT L_c=12.

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

QMC $T = 0.05t < \omega_0$

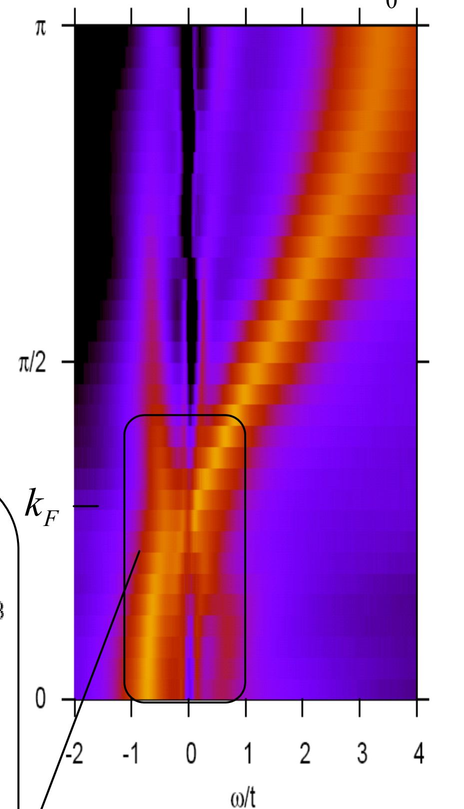


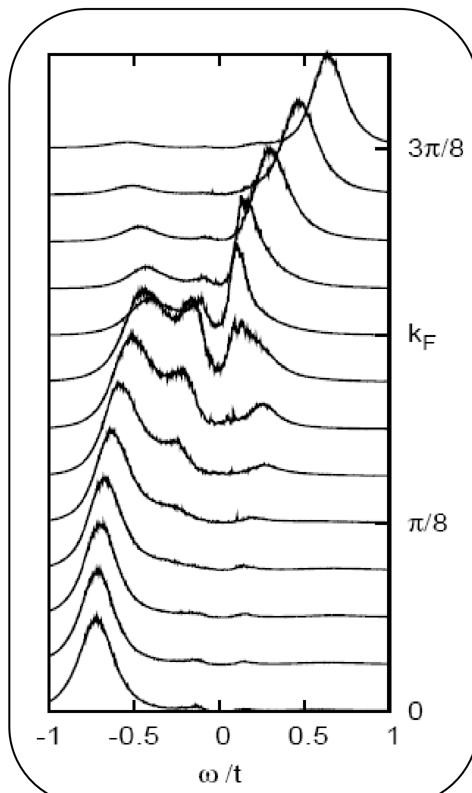


<u>Interpretation:</u>
Breaking of a bipolaron.
Energy cost is the spin gap:
$\Delta_{sp} \sim 0.2t \sim 2\Delta_{qp}$

Consistent with Luther-Emery liquid.

QMC $T = 0.025t < \omega_0$

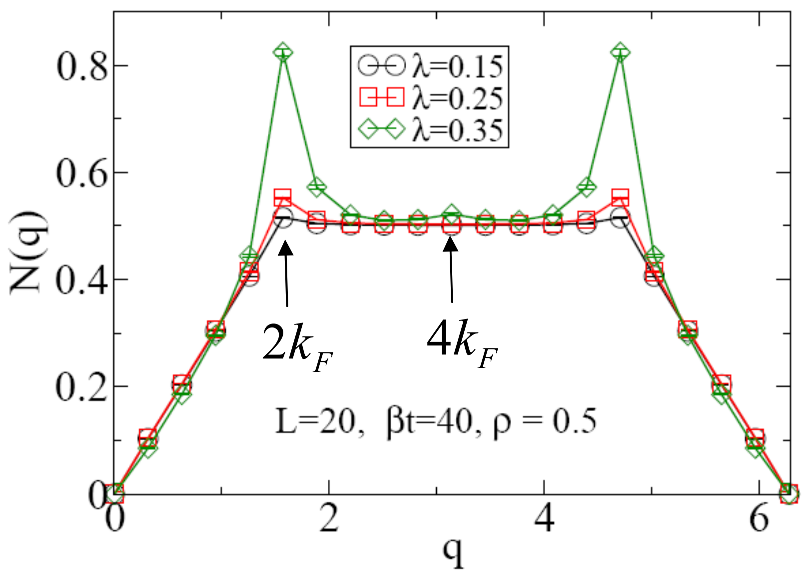




Luttinger Liquid, λ=0.15, 0.25

$$\langle n(\boldsymbol{r})n(\boldsymbol{0})\rangle = \frac{K_\rho}{(\pi \boldsymbol{r})^2} + A_1 \cos(2\boldsymbol{k}_f \boldsymbol{r})\boldsymbol{r}^{-1-K_\rho} + \cdots$$
$$+A_2 \cos(4\boldsymbol{k}_f \boldsymbol{r})\boldsymbol{r}^{-4K_\rho}$$
$$\langle \boldsymbol{S}(\boldsymbol{r})\boldsymbol{S}(\boldsymbol{0})\rangle = \frac{1}{(\pi \boldsymbol{r})^2} + B_1 \cos(2\boldsymbol{k}_f \boldsymbol{r})\boldsymbol{r}^{-1-K_\rho} + \cdots$$
$$\langle \Delta^\dagger(\boldsymbol{r})\Delta(\boldsymbol{0})\rangle = C\boldsymbol{r}^{-1-1/K_\rho} + \cdots$$

$$\boxed{K_\rho = \pi \lim_{\boldsymbol{q}\to 0} \frac{\mathrm{d}N(\boldsymbol{q})}{\mathrm{d}\boldsymbol{q}}}$$

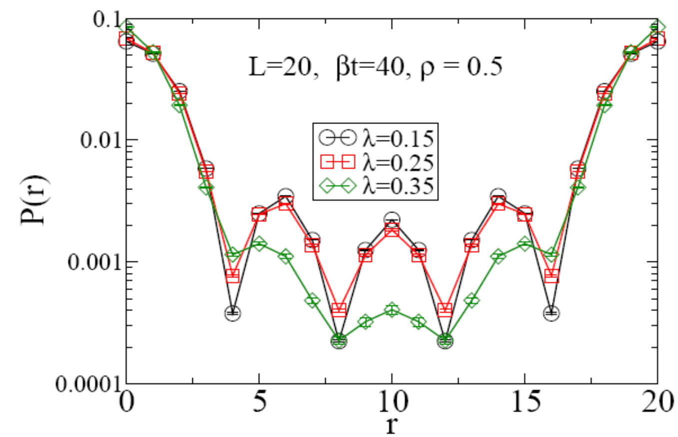


→ $K_\rho = 1.0341 \pm 0.0006$ at $\lambda = 0.15$
$K_\rho = 1.0441 \pm 0.0002$ at $\lambda = 0.25$

Luther-Emery Liquid, λ=0.35

$$\langle n(\boldsymbol{r})n(\boldsymbol{0})\rangle = \frac{A_0}{\boldsymbol{r}^2} + A_1 \cos(2\boldsymbol{k}_f \boldsymbol{r})\boldsymbol{r}^{-K_\rho} + \cdots$$
$$+A_2 \cos(4\boldsymbol{k}_f \boldsymbol{r})\boldsymbol{r}^{-4K_\rho}$$
$$\langle \Delta^\dagger(\boldsymbol{r})\Delta(\boldsymbol{0})\rangle = C\boldsymbol{r}^{-1/K_\rho} + \cdots$$

Dominant $2k_f$ charge → Kρ<1



Pairing correlations fall of quicker than $1/r^2$ → Kρ<1/2

Summary.

Weak-coupling CT-QMC.

- Simple and flexible method. Perfectly suited for cluster methods (DCA, CDMFT)
- Allows to acces "large" clusters.
- Projective schemes ✓
- Generalization to include phonons. ✓

¼ Filled Holstein model .

Luttinger Liquid.

Peierls phase.
Bipolaronic CDW.

λ_c λ

Gapless spin
Gapless charge.

Gapfull spin
Gapless charge.
→ Luther-Emery.

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