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Optical conductivity in the Hubbard model in the limit $d \to \infty$

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9.12.98

$$\sigma(\omega) = 0$$

all transport properties vanish for $d \to \infty$

solution: consider $d \cdot \sigma(\omega)$

Experiments, Connection to reflectivity

Theory:
- $\sigma(\omega)$ in lattice models
- $\sigma(\omega)$ in $d=\infty$: $\sigma = \sigma\{\Sigma\}$

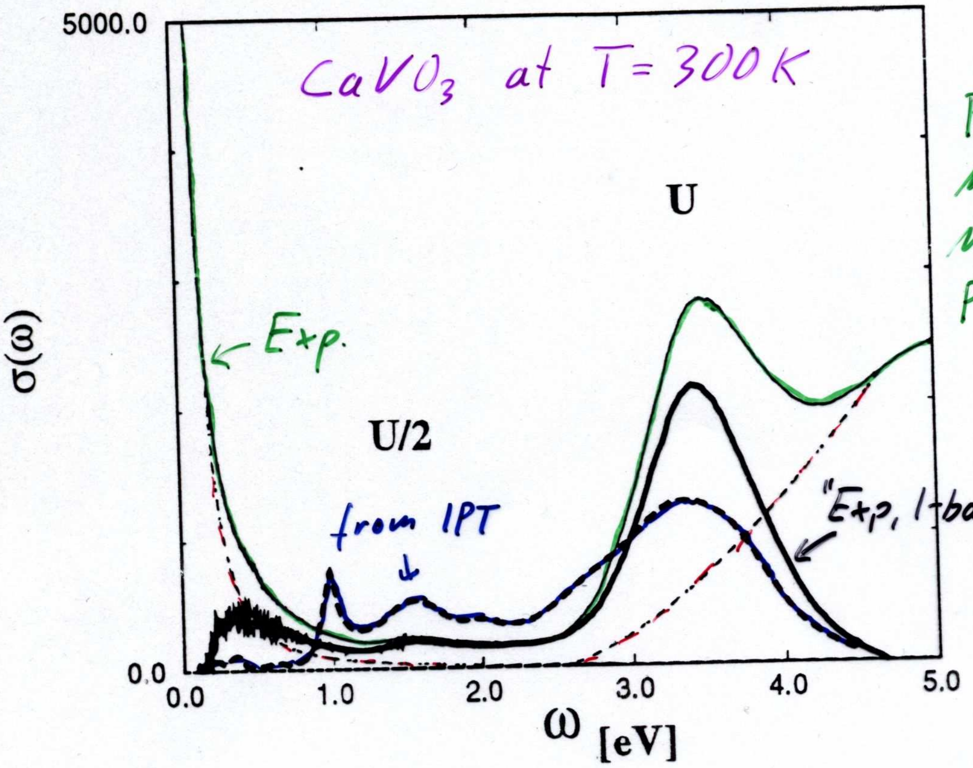
Practice: numerical calculation of $\sigma(\omega)$

Tests, Results

Problems, Outlook

Conclusion

Experiments, Connection to reflectivity



Rozenberg, Inoue, Makino, Iga, Nishihara PRL 76, 4781 (1996)

$$\vec{j}(\omega) = \sigma(\omega)\,\vec{E}(\omega) \quad \text{(isotropic case)}$$

complex

$$\varepsilon(\omega) = \varepsilon_0(\omega) + \frac{4\pi i\,\sigma(\omega)}{\omega} \quad \text{dielectric constant}$$

$$r = \left|\frac{1-k}{1+k}\right|^2 = \frac{(1-n)^2+k^2}{(1+n)^2+k^2}\ ; \quad k = \sqrt{\varepsilon} =: n + ik$$

related by Kramers-Kronig

Theory

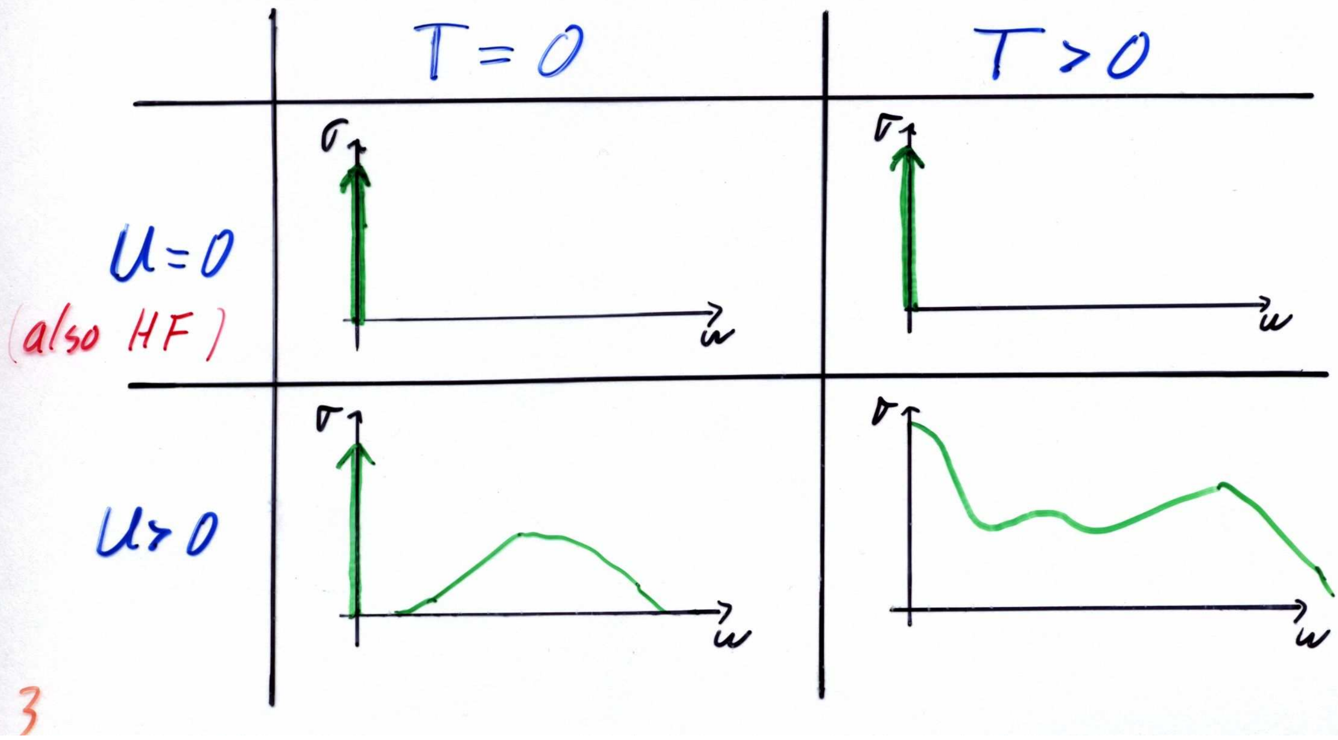
current operator $\vec{j}_{\vec{k}} = e \vec{v}_{\vec{k}} \hat{n}_{\vec{k}}$; $\vec{v}_{\vec{k}} = \frac{1}{\hbar} \nabla_{\vec{k}} \varepsilon_{\vec{k}}$

if $[\hat{H}, \hat{n}_{\vec{k}}] = 0 \Rightarrow \vec{j} := \sum_{\vec{k}} \langle \vec{j}_{\vec{k}} \rangle$ time independent,
no dissipation
$\sigma(\omega) \propto \delta(\omega)$

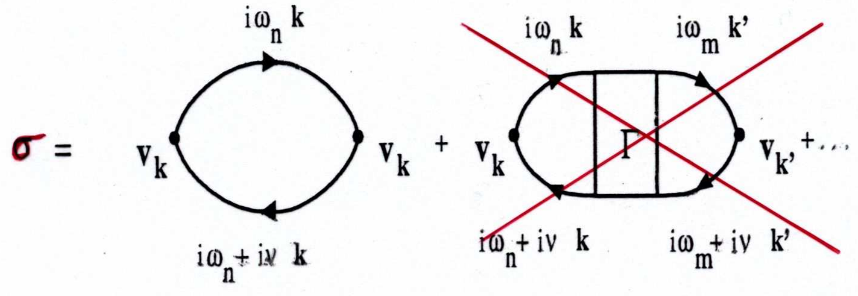
fluctuation-dissipation theorem:

$$\boxed{\begin{aligned} d\sigma(\omega) &= \frac{1}{N} \frac{1}{i(\omega+i\delta)} \sum_{l} \langle\langle j_l, j_l \rangle\rangle (\underbrace{\omega+i\delta}_{z}) \\ &= \frac{1}{iz} \frac{1}{N} \sum_{k,k',\sigma} \sum_{l} v_{k_l} v_{k'_l} \langle\langle n_{k\sigma}, n_{k'\sigma} \rangle\rangle (z) \end{aligned}}$$

qualitative behavior in Hubbard model:



simplifications in the limit $d \to \infty$:



momentum factorizes, odd parity

Khurana, PRL 64, 1990 (1990): $\sigma(\omega)$ functional of $\Sigma(\omega)$, no vertex corrections

Schweitzer, Czycholl, PRL 67, 3724 (1991): $\sigma(\omega=0) = \sum_{R,R',k,k',\sigma} \int d\varepsilon \ldots$ for PAM

Pruschke, Cox, Jarrell, PRB 47, 3553 (1993):

free DOS; fermi function

$$d\,\sigma(\omega) = \pi \int d\omega' \int d\varepsilon \, \boxed{A_0(\varepsilon)} \, A(\varepsilon,\omega') A(\varepsilon,\omega'+\omega) \frac{f(\omega')-f(\omega'+\omega)}{\omega}$$

for hc lattice with NN hopping; $A(\varepsilon,\omega) = \mathrm{Im} \frac{1}{\omega - \varepsilon - \boxed{\Sigma(\omega)} + i\delta}$

Rozenberg, Kotliar, Kajueter, Thomas, Rapkine, Honig, Metcalf, PRL 75, 105 (1995): application to Bethe lattice with NNN hopping

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sum rules: Drude weight $D_{non} \overset{T=0}{=} \pi \rho(\varepsilon_F)$; $D_{FL} \overset{T=0}{=} \frac{\pi}{m^*/m} \rho(\varepsilon_F)$

f-sum rule $2\int_0^\infty \sigma(\omega)\, d\omega = -\pi \langle E_{kin} \rangle$?

Practice

$\Sigma(\omega)$ from
- NCA Pruschke et al, PRB 47, 3553 (1993)
- IPT, ED Rozenberg et al, PRL 75, 105 (1995)
- QMC + annealing Jarrel, Freericks, Pruschke, PRB 51, 11704 (1995)

computation of $\sigma(\omega)$ from QMC:

QMC $\longrightarrow \{G_i(\tau)\}$

average $\Downarrow$

$G(\tau), \Delta G(\tau)$ loss of information

MEM $\Downarrow$ $\quad G(\tau) = \int d\omega \, \frac{e^{-\tau\omega}}{1+e^{-\beta\omega}} \, \overbrace{\frac{\mathrm{Im}\, G(\omega)}{-\pi}}^{A(\omega)}$ ill conditioned

$\mathrm{Im}\, G(\omega)$

Kramers Kronig $\Downarrow$ $\quad \mathrm{Re}\, G(\omega) = -\frac{1}{\pi} P \int_{-\infty}^{\infty} d\omega' \, \frac{\mathrm{Im}\, G(\omega')}{\omega - \omega'}$

$G(\omega)$

inv. Dyson Eq. $\Downarrow$ $\quad G(\omega) = \int d\varepsilon \, \frac{\rho_0(\varepsilon)}{\omega - \varepsilon - \Sigma(\omega)}$ easy for Bethe DOS

$\Sigma(\omega)$

numerical Integration $\Downarrow$ $\longleftarrow$ requires analyticity ($\mathrm{Im}\, \Sigma(\omega) \le 0$)

$\sigma(\omega)$

problem: numerics may violate analyticity, especially in AB phases

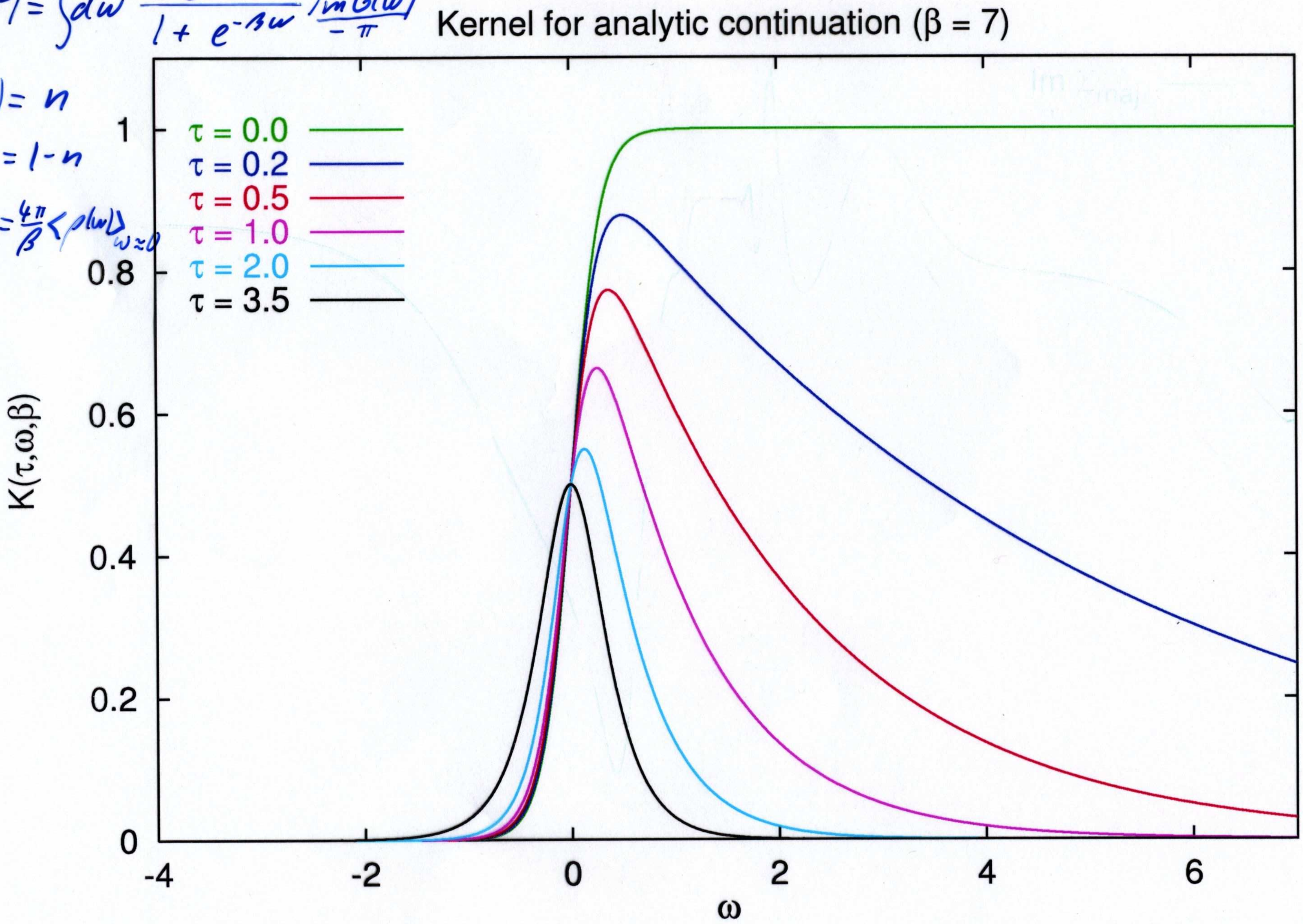
critical step: maximum entropy method (MEM)
- tries to find most probable (smooth) $G(\omega)$ compatible w. $G(\tau)$
- (additional physical input: default model, enforce analyticity)

$$G(\tau) = \int d\omega \, \frac{e^{-\tau\omega}}{1 + e^{-\beta\omega}} \frac{\operatorname{Im} G(\omega)}{-\pi}$$

$G(\beta) = n$

$G(0) = 1 - n$

$G\left(\frac{\beta}{2}\right) = \frac{4\pi}{\beta} \langle \rho(\omega) \rangle_{\omega \approx 0}$



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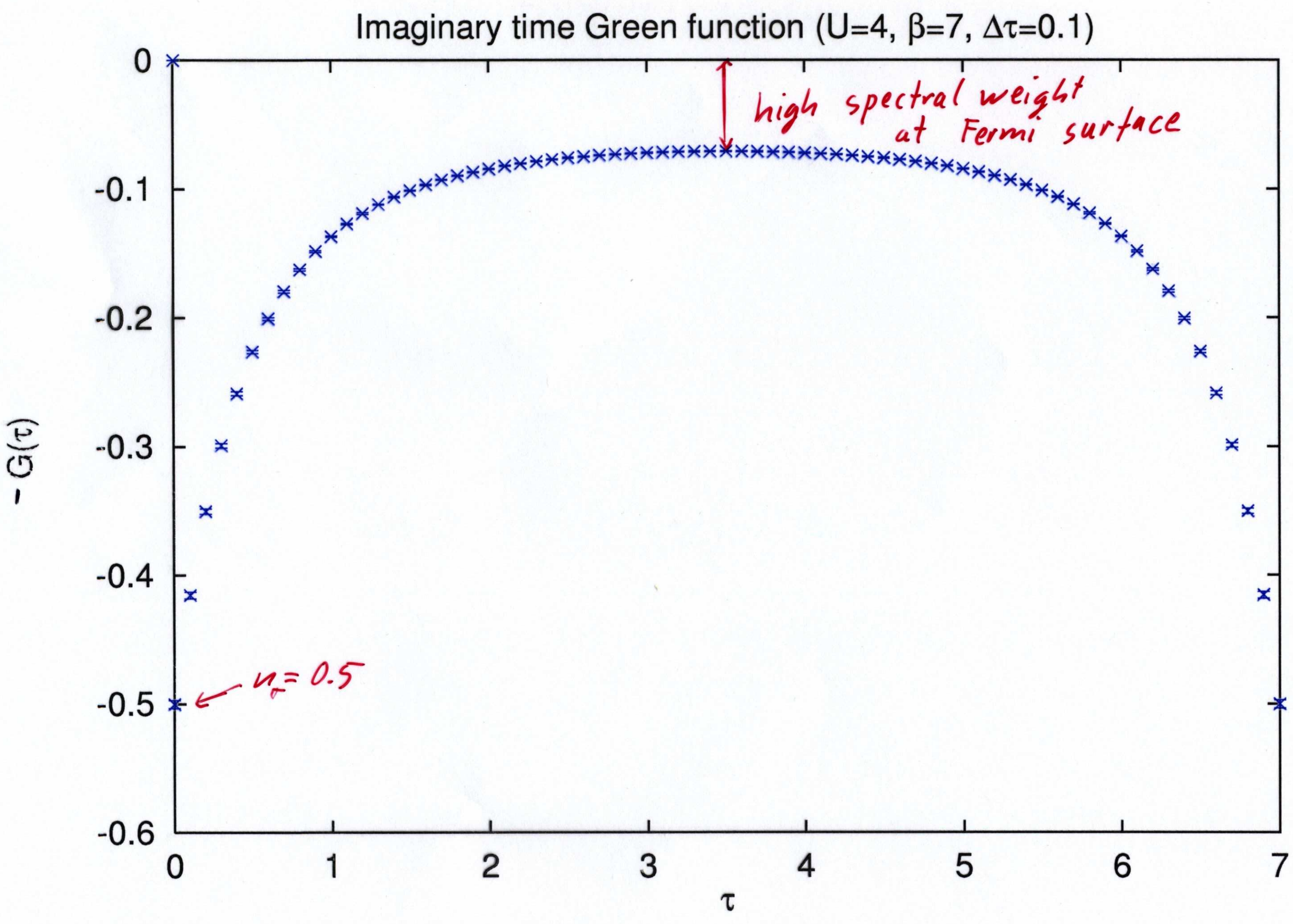
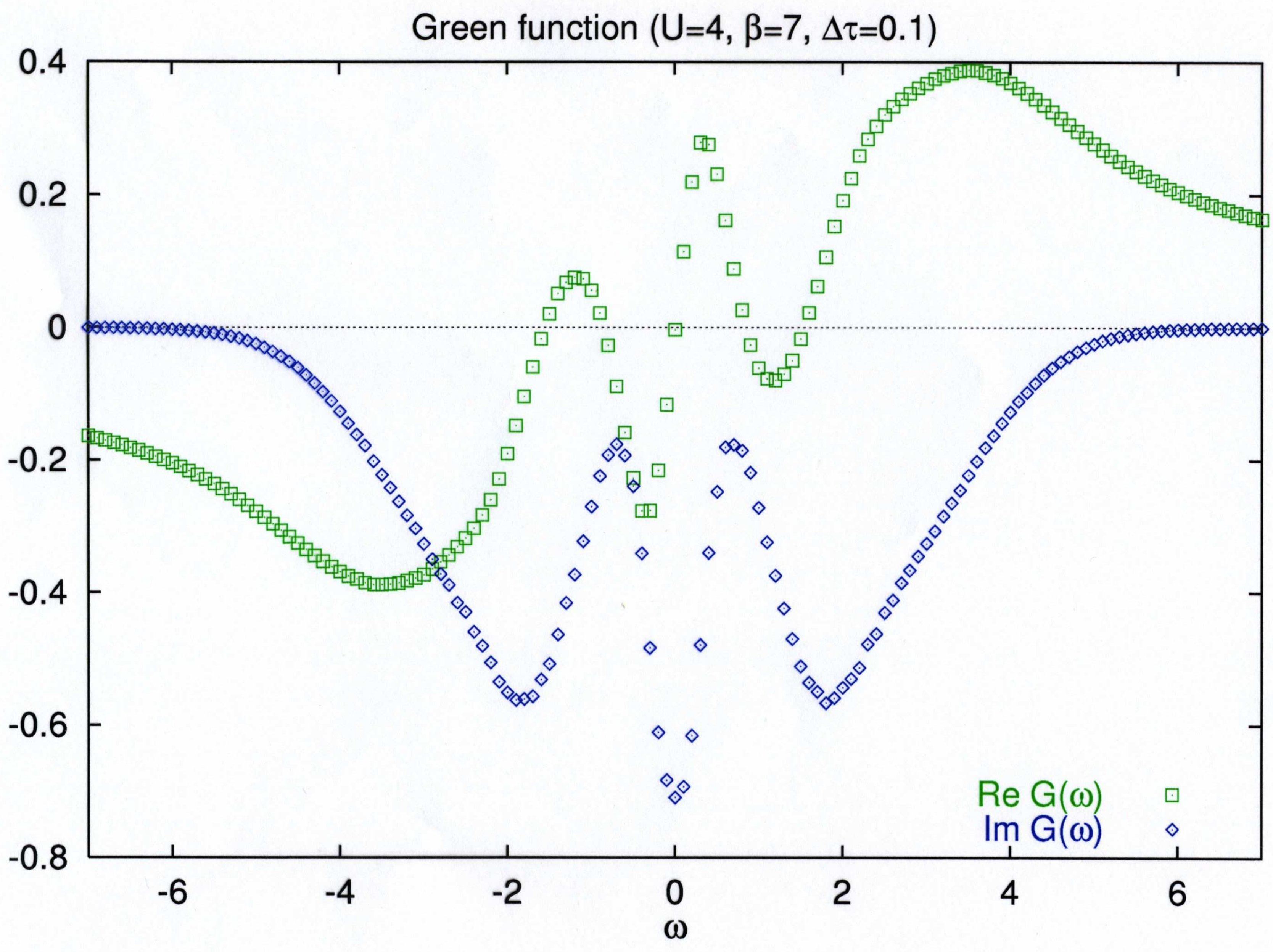
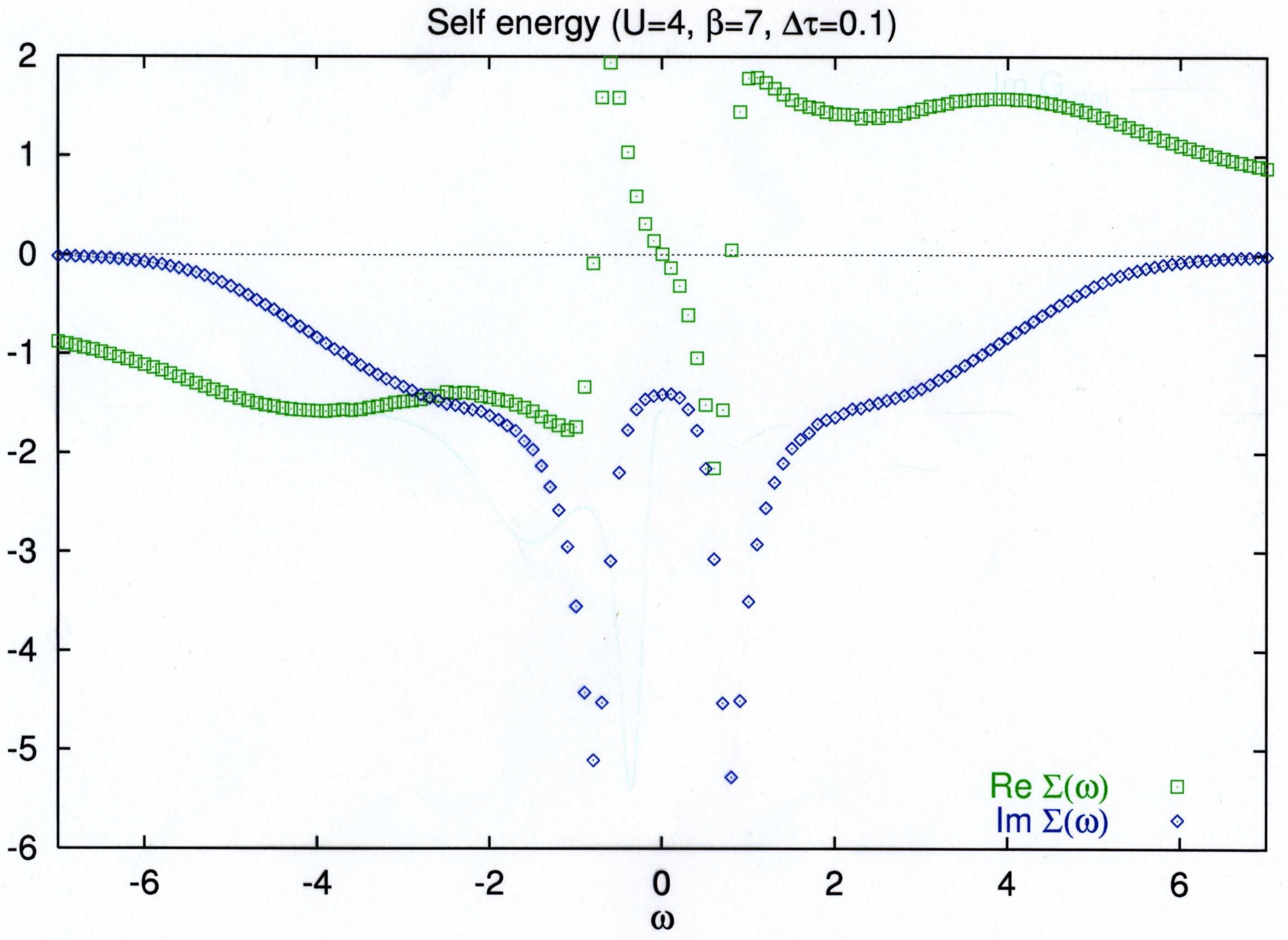


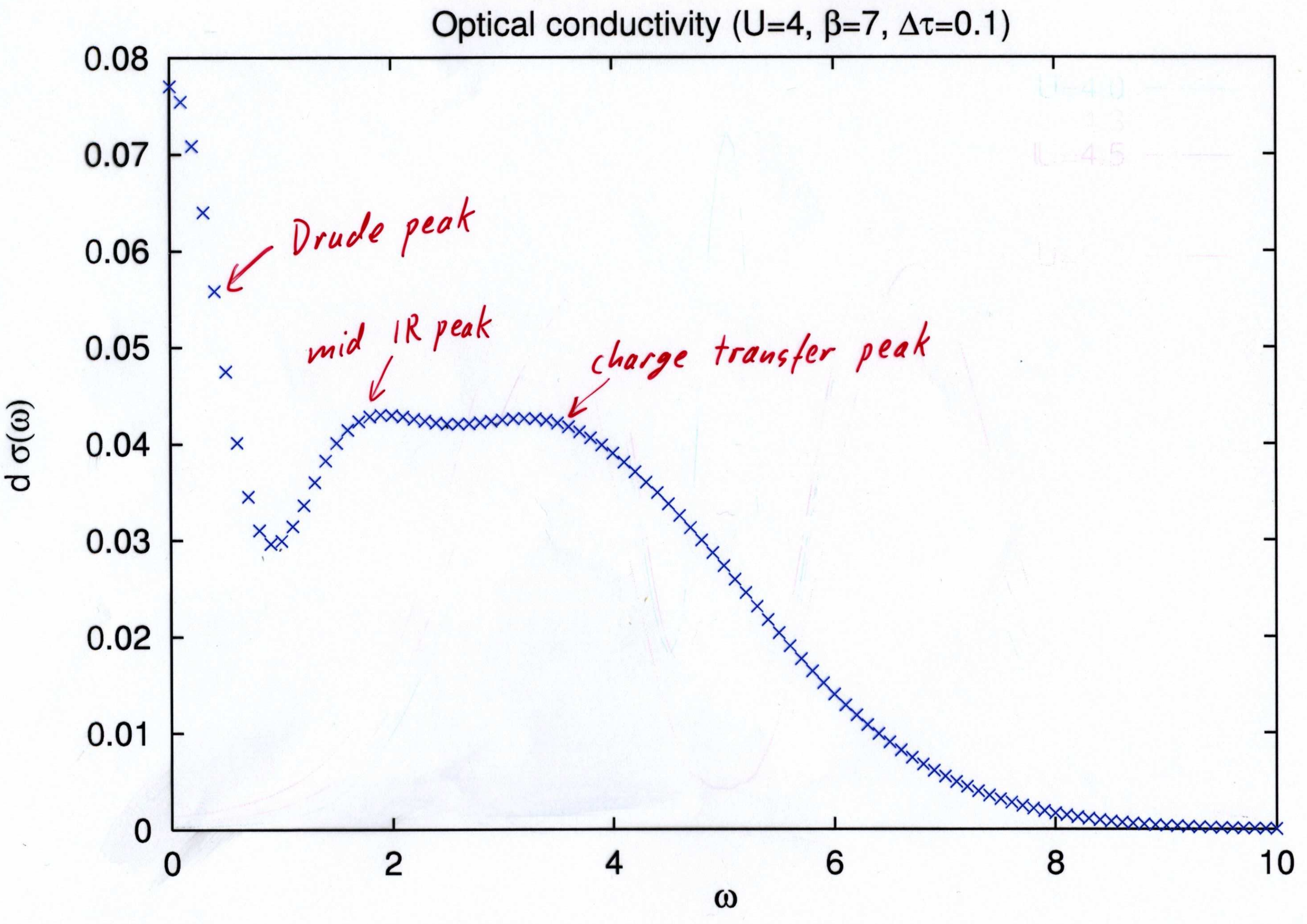
Imaginary time Green function (U=4, β=7, Δτ=0.1)
high spectral weight at Fermi surface
$n_\sigma = 0.5$
- G(τ)
τ
0
-0.1
-0.2
-0.3
-0.4
-0.5
-0.6
0
1
2
3
4
5
6
7

(8)


Green function (U=4, β=7, Δτ=0.1)
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
-6
-4
-2
0
2
4
6
ω
Re G(ω)
Im G(ω)

(9)




Optical conductivity (U=4, β=7, Δτ=0.1)
d σ(ω)
ω
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
0
2
4
6
8
10
Drude peak
mid IR peak
charge transfer peak

Tests, Results

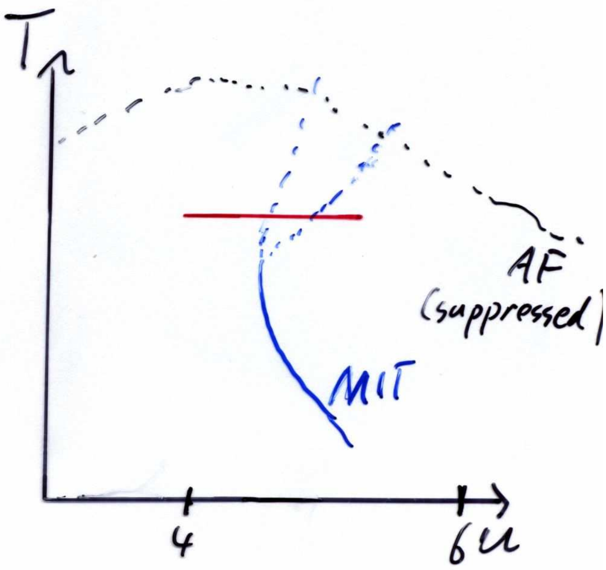
1. $U=0 \Rightarrow \Sigma(\omega)=0 \Rightarrow \sigma(\omega) \propto \delta(\omega)$

in practice: • finite grid, here $\Delta\omega = 0.01$

• finite broadening δ

works as long as $\delta \gtrsim \frac{\Delta\omega}{2}$

2. metal-insulator transition at half filling, relatively high temperature $T=\frac{1}{7}$



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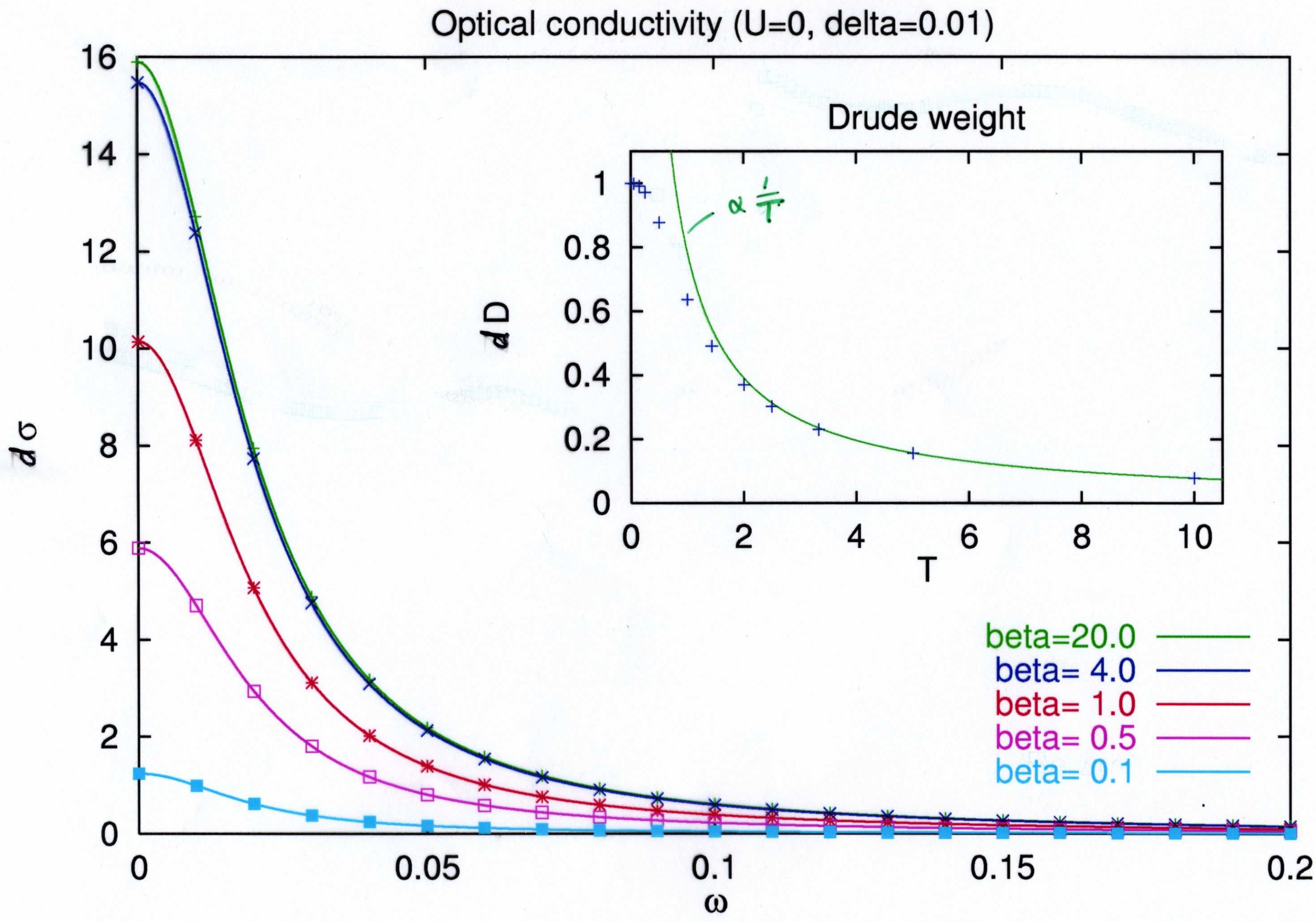

Optical conductivity (U=0, delta=0.01)
Drude weight
$\propto \frac{1}{T}$
$d\mathrm{D}$
T
$d\sigma$
ω
beta=20.0
beta= 4.0
beta= 1.0
beta= 0.5
beta= 0.1

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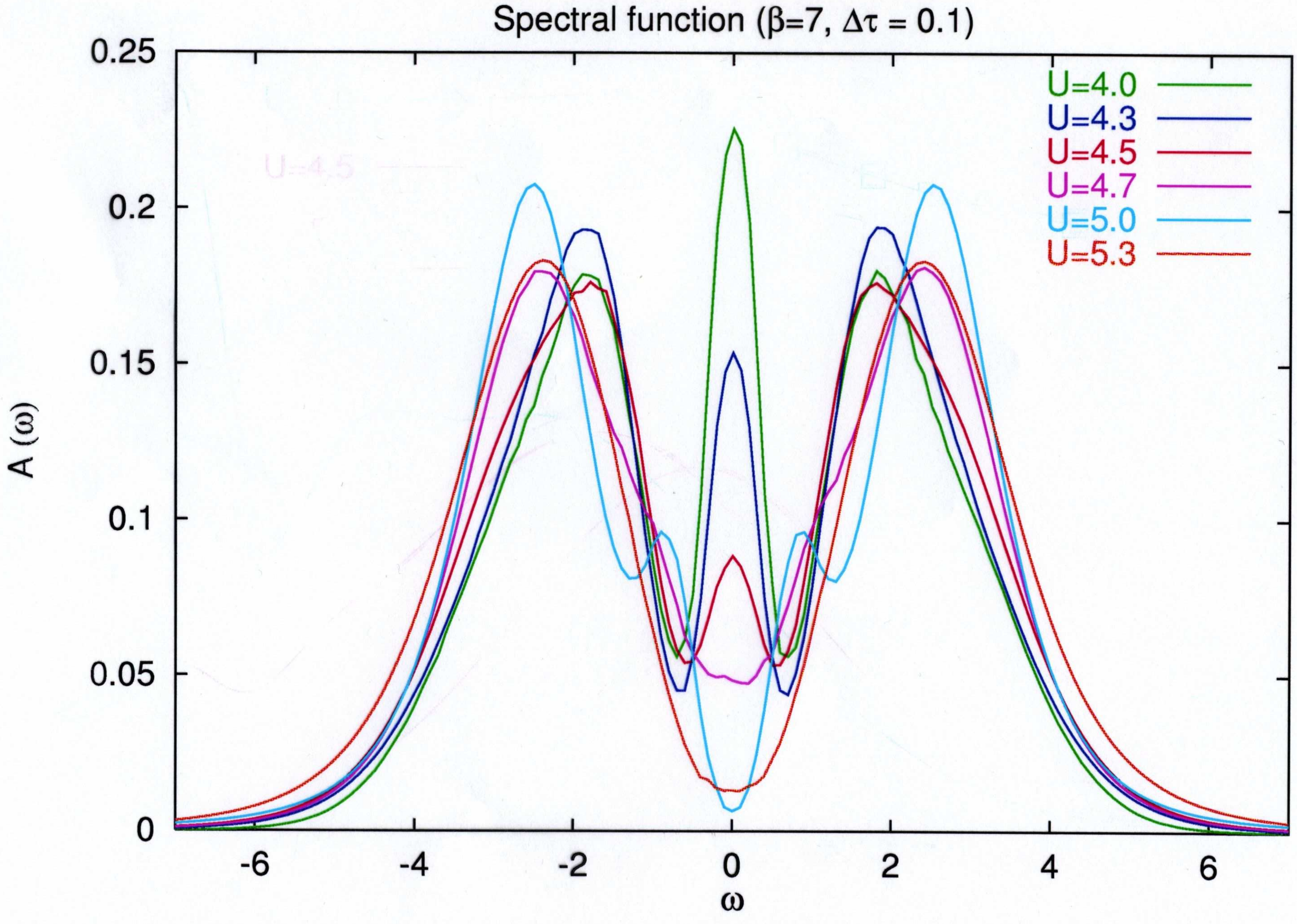
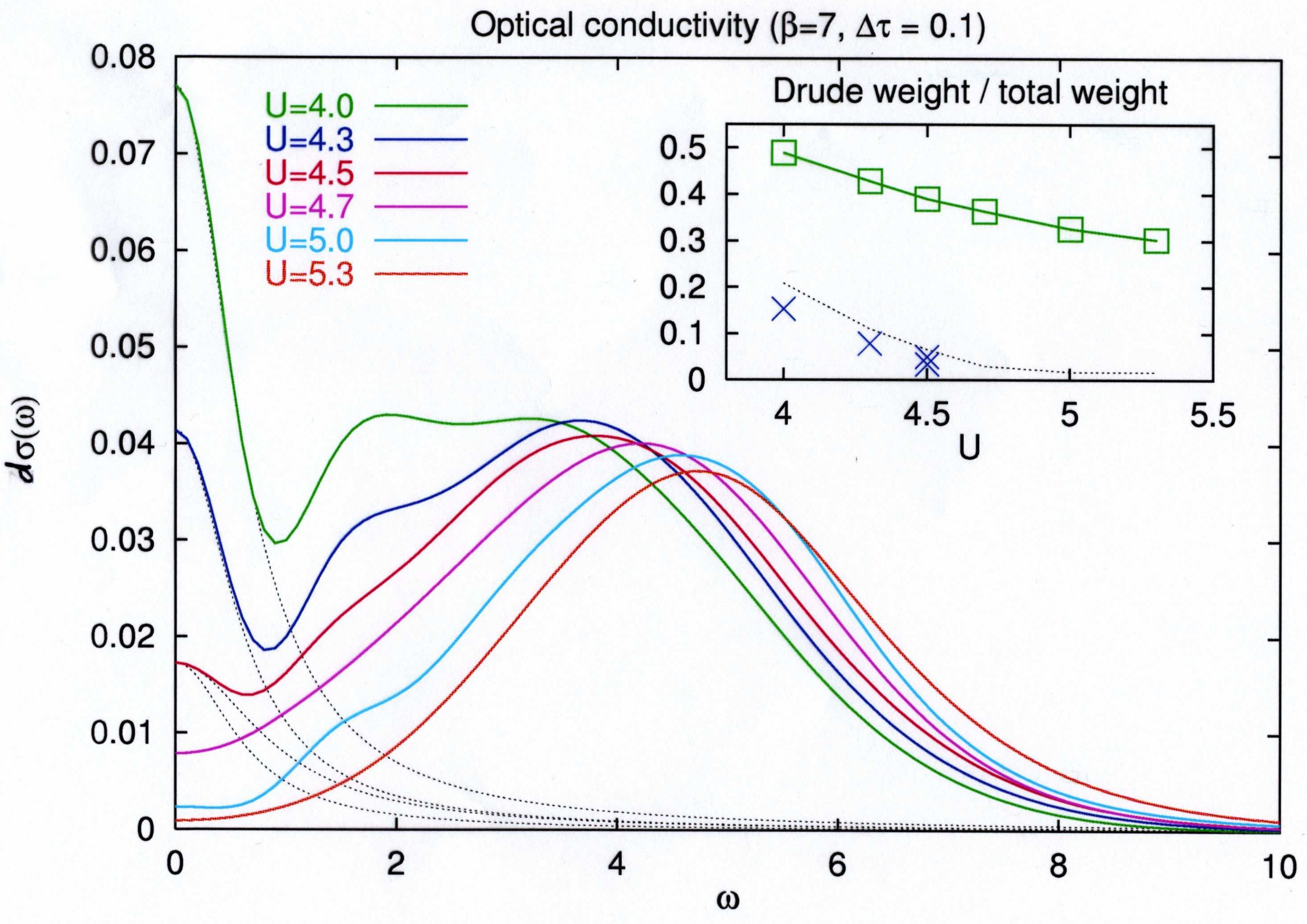


Spectral function (β=7, Δτ = 0.1)
A (ω)
ω
0.25
0.2
0.15
0.1
0.05
0
-6
-4
-2
0
2
4
6
U=4.0
U=4.3
U=4.5
U=4.7
U=5.0
U=5.3

(14)


Optical conductivity (β=7, Δτ = 0.1)
U=4.0
U=4.3
U=4.5
U=4.7
U=5.0
U=5.3
Drude weight / total weight
0.5
0.4
0.3
0.2
0.1
0
4
4.5
5
5.5
U
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
σ(ω)
0
2
4
6
8
10
ω

Problems, outlook

1. analyticity: for Bethe DOS: $\Sigma_\alpha(\omega) = \omega + \mu - (G_\alpha(\omega))^{-1} - \frac{D^2}{4} G_{\bar\alpha}(\omega)$

   sub-lattice index

   set $D=2$: $\mathrm{Im}\,\Sigma_\alpha(\omega) = \frac{\mathrm{Im}\,G_\alpha(\omega)}{|G_\alpha(\omega)|^2} - \mathrm{Im}\,G_{\bar\alpha}(\omega) \overset{!}{\leq} 0$

   $$\Downarrow$$

   $$\frac{\mathrm{Im}\,G_\alpha}{\mathrm{Im}\,G_{\bar\alpha}} \geq \mathrm{Re}\,G_\alpha^2 + \mathrm{Im}\,G_\alpha^2$$

   $$\mathrm{Re}\,G_\alpha^2 \geq 0 \quad \Downarrow \quad \mathrm{Im}\,G_\alpha^2 \geq 0$$

   $$\boxed{\mathrm{Im}\,G_\alpha\,\mathrm{Im}\,G_{\bar\alpha} \leq 1; \quad \frac{\mathrm{Im}\,G_\alpha}{\mathrm{Im}\,G_{\bar\alpha}} \geq \mathrm{Re}\,G_\alpha^2}$$

   requires Kramers-Kronig (avoidable by coarse-graining)

   enforce within MEM ⇒
   - $\Sigma(\omega)$ available
   - $\mathrm{Im}\,G(\omega)$ <u>more</u> reliable

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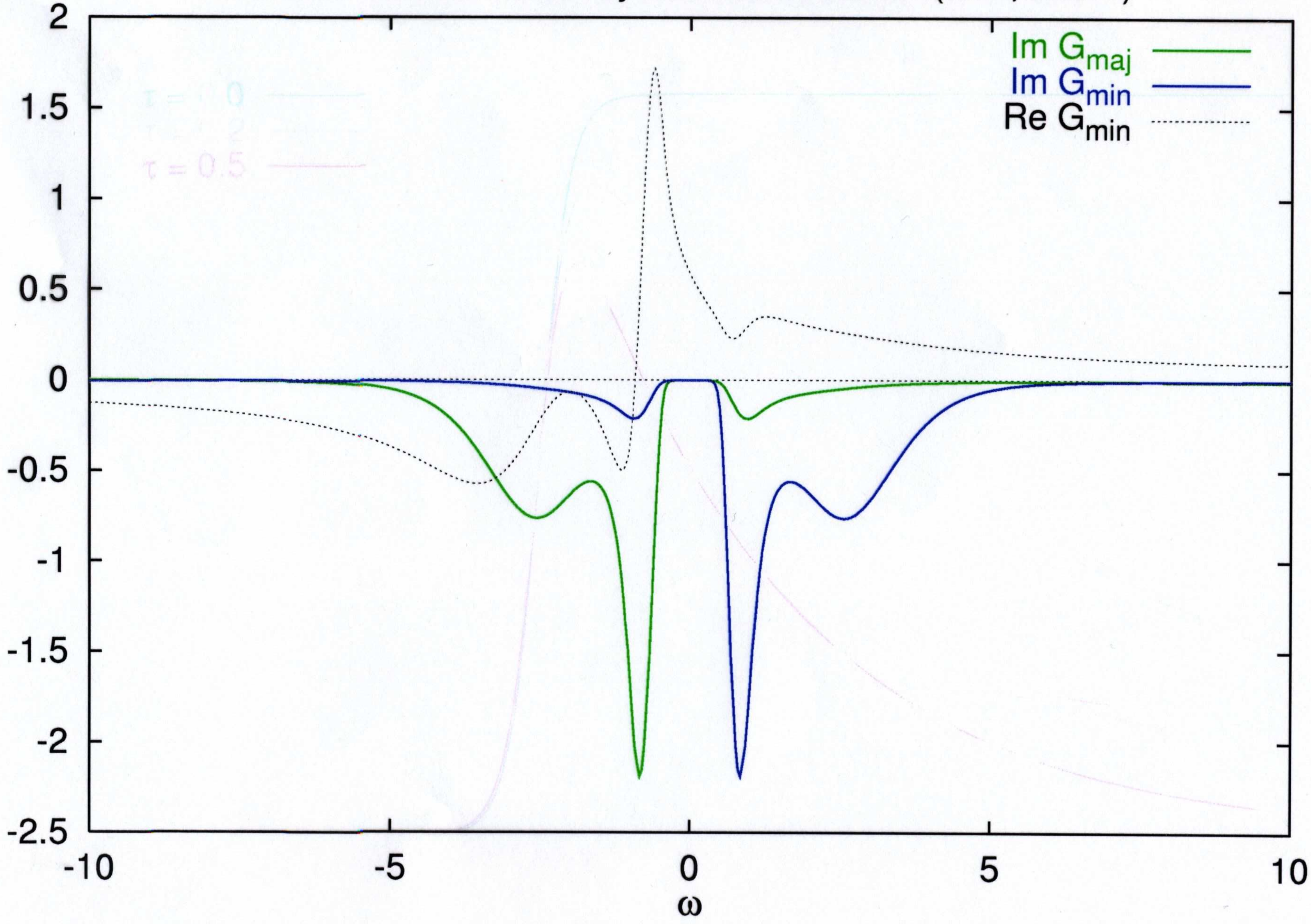
2. use up-to-date MEM (M. Jarrell), test default models (started)
3. test "conditioning" within QMC (from M. Ulmke + M. Jarrell)
4. generalize to asymmetric model DOS

Green function for AF system with disorder (U=4, Δ=0.1)



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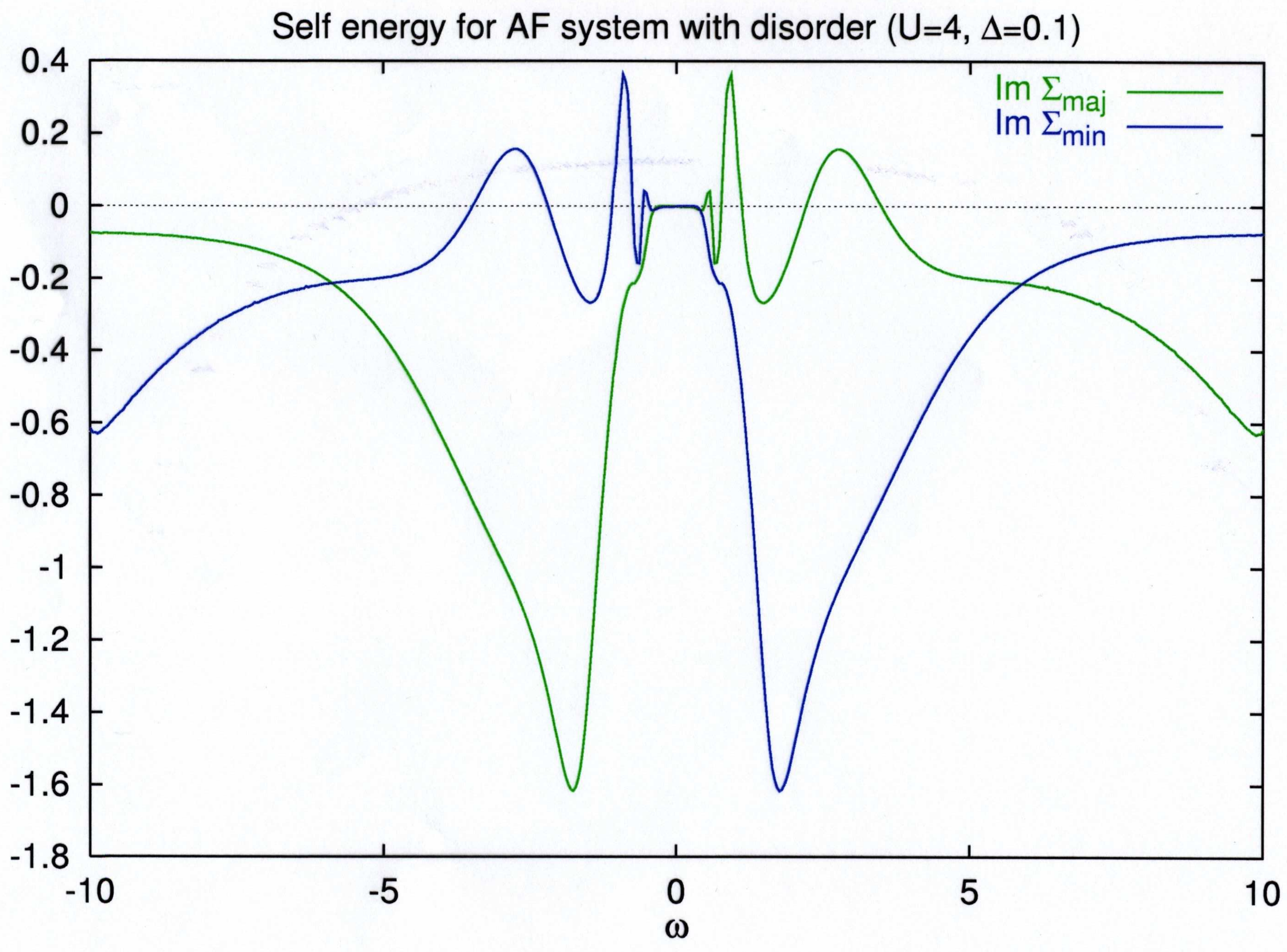

Self energy for AF system with disorder (U=4, Δ=0.1)
Im Σmaj
Im Σmin
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
-1
-1.2
-1.4
-1.6
-1.8
-10
-5
0
5
10
ω

Conclusion

$\sigma(\omega)$: • interesting physical property from microscopic theory

• provides checks for more basic properties

Main practical problem is reliable $\mathrm{Im}\, G(\omega)$ (QMC, MEM)

Beyond 1-band: additional high-energy features

Beyond $d=\infty$: normal scattering from vertex corrections reduces importance of umklapp processes
$\rightsquigarrow$ increase of $\sigma(\omega)$ expected

Beyond Hubbard model: electron-phonon interaction + impurities $\rightsquigarrow$ broadening