The f-electron spectrum of the Falicov-Kimball model near a quantum-critical point

J. K. Freericks, V. Turkowski, and V. Zlatic

Department of Physics

Georgetown University

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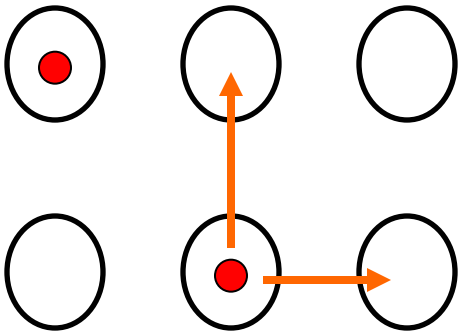
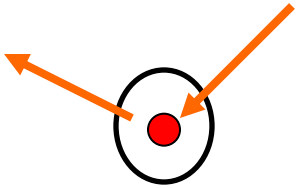
Dynamical mean field theory

- Models of strongly correlated materials are difficult to solve.
- Significant progress has been made over the past 15 years by examining the limit of **large spatial dimensions**.
- In this case, the lattice problem can be mapped onto a self-consistent impurity (single-site) problem, in a time-dependent field that **mimics the hopping of electrons onto and off of the lattice sites**.

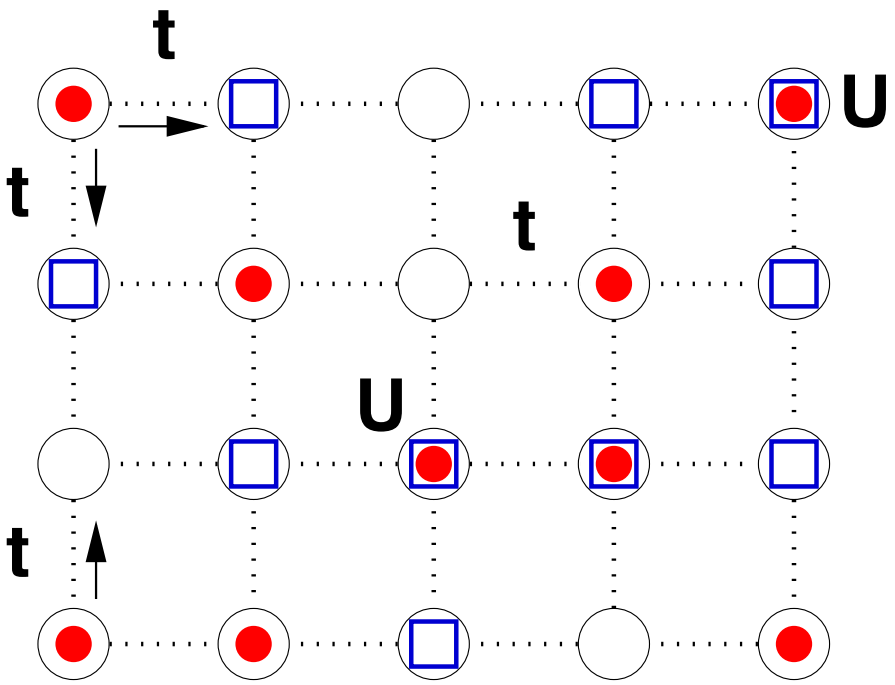


Lattice



Impurity site

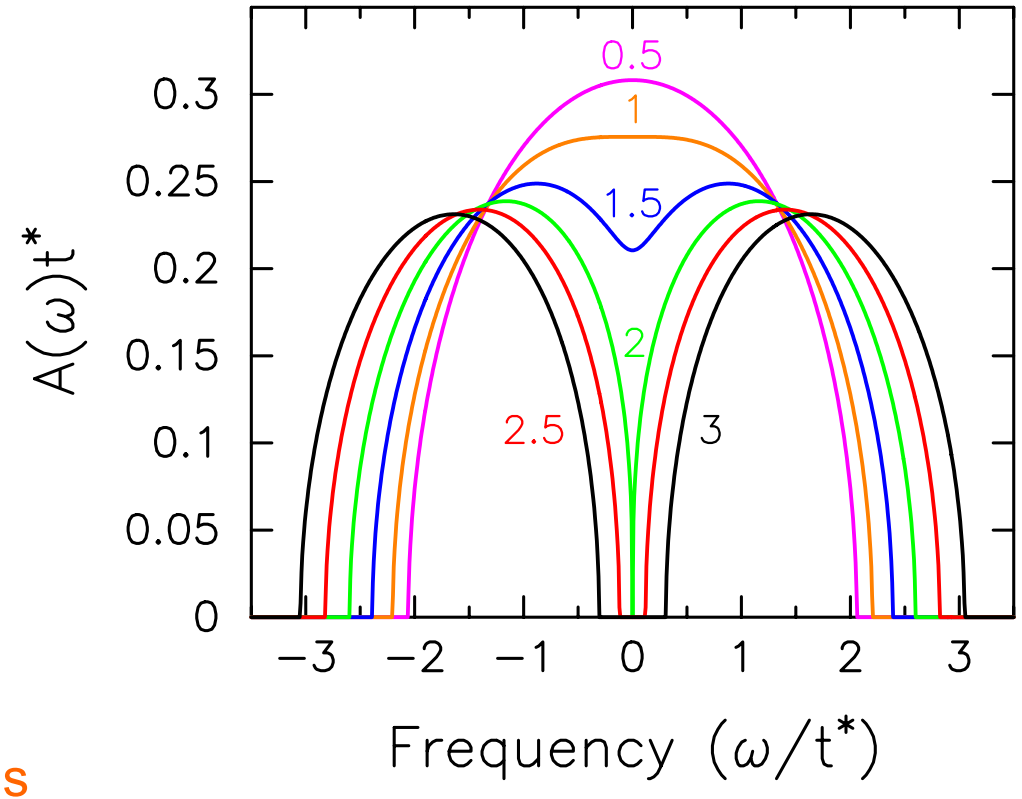
Falicov-Kimball Model



- Two kinds of particles: (i) **mobile electrons** and (ii) **localized electrons**.
- When both electrons are on the same site they interact with a correlation energy U.
- Many-body physics enters from an **annealed average over all localized electron configurations**.

DOS (conduction electrons)

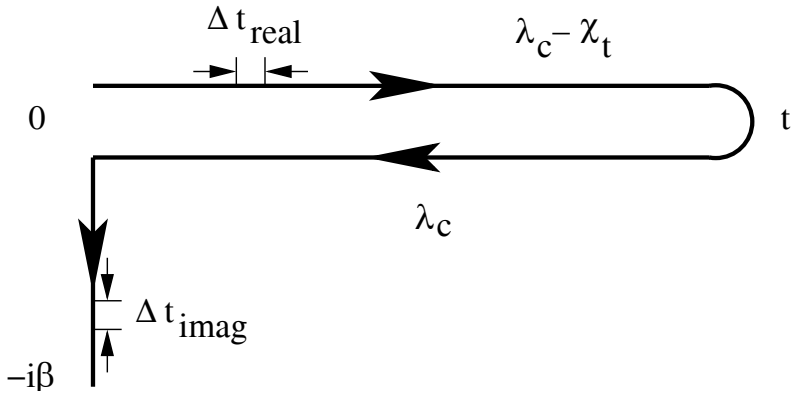
- The Falicov-Kimball model is **not** a Fermi liquid.
- On a Bethe lattice, it has a **Mott transition** at U=2 and half filling.
- The conduction-electron DOS is **independent of temperature**, and **continuously decreases to zero** at the chemical potential as U increases. Then a **true gap forms** which increases with U.
- On the **hypercubic lattice**, it is a **pseudogap** that occurs for U>√2.



DOS (localized electrons)

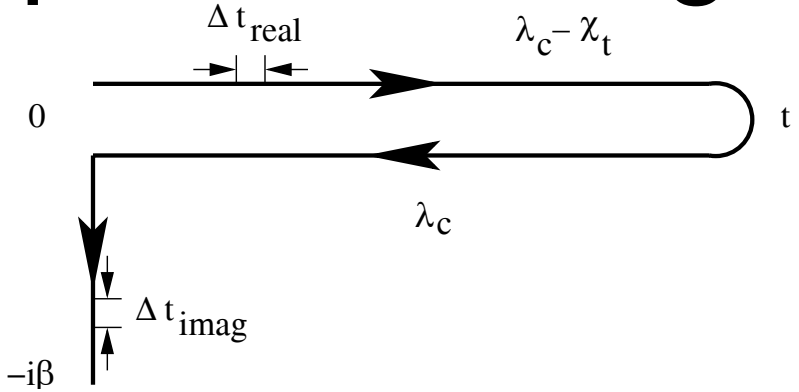
- The localized electrons **interact** with the conduction electrons when they sit on the same lattice site.
- Since the hopping of the conduction electrons on the lattice is mimicked by a time-dependent field (called λ) for the impurity, the localized electrons **feel an additional time-dependent field** (called χ) when the conduction electrons are sitting on the impurity site.
- The first time dependent field $\lambda(t,t')$ is a function of **the difference of the time coordinates** (and measures the probability for a conduction electron to hop onto the site at time t and hop off at time t'), while the second field $\chi(t,t')$ is proportional to a delta function in t-t', but **multiplied by a function of time**.
- ***Hence there is no overall time-translation invariance for the localized electrons.***

Keldysh formalism



- Problems without time-translation invariance can be solved with a so-called **Keldysh formalism**.
- Green's functions are defined with time arguments that run over the **Kadanoff-Baym contour**.
- The electrons evolve in the fields **forwards** in time, then de-evolve in the fields **backwards** in time.
- **Functional derivatives** are then used to determine the Green's functions and other correlation functions of interest.

Computational Algorithm



- The key element in calculating the real-time Green's function is to calculate the **Feynman determinant of a continuous integral operator** defined on the Kadanoff-Baym contour.
- This operator is first **discretized** on a grid to be represented by **finite-dimensional** matrices.
- The matrix varies for each value of time (both in size and in its matrix elements).
- Hence we need to **generate**, and **calculate the determinant** of a large number (approximately 500) **general complex matrices** of size up to about 2500X2500.
- Since the only information needed to generate the matrices is the dynamical mean field λ, the interaction strength U, and the temperature, **this procedure is easily parallelized**.

Parallel implementation

(1) **Solve** for the conduction electron Green's function to determine the **dynamical mean field** λ on the **master node**.
(2) **Broadcast** the field $\lambda(t,t')$, the interaction U, and the temperature T to **all slave nodes**.
(3) **Send** each **slave node** a value of time to calculate the Green's function at that time. This involves generating a matrix and calculating its determinant. (LAPACK routines are used for efficiency.)
(4) **Send** data back to the **master** for storage; **repeat** for a new value of time.
(5) **Process** the real-time data to construct the Fourier transform, and **extract** the interacting DOS of the localized electrons.

Numerical issues

- The Green's function decays exponentially in time, so we need to compute the real time Green's function out to **long enough times** where it becomes small enough that **it can be neglected for larger times in the Fourier transforms**.
- The systematic error associated with the discretization size on the real time axis **affects the rate of decay** of the Green's function at long times and this error **increases as the temperature is reduced**.
- The long-time tails **develop oscillatory components** when the interaction strength is large enough, **precluding an extrapolation out to large times**.
- A number of different extrapolation schemes exist to try to reduce the discretization size to zero on the real-time axis. **Criteria need to be developed to choose the best extrapolation**.

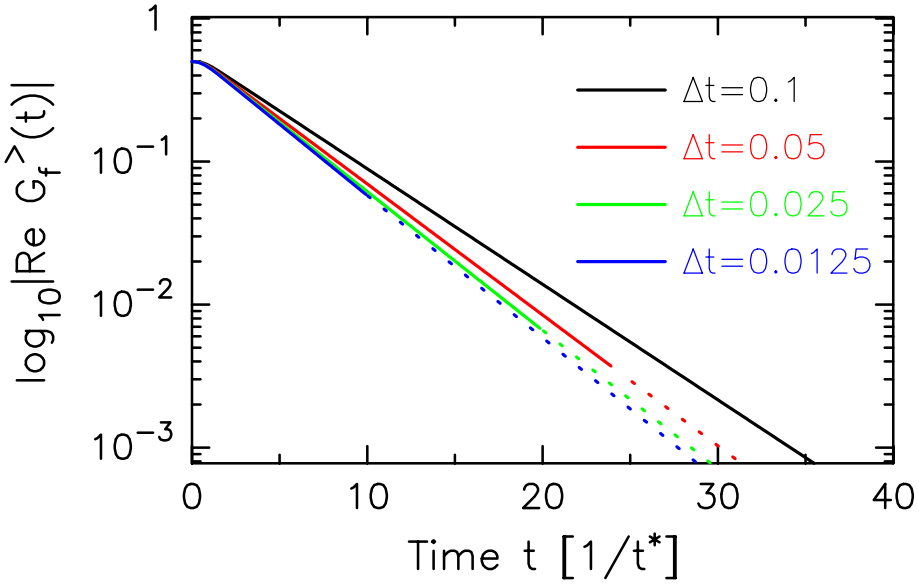
Sum rules

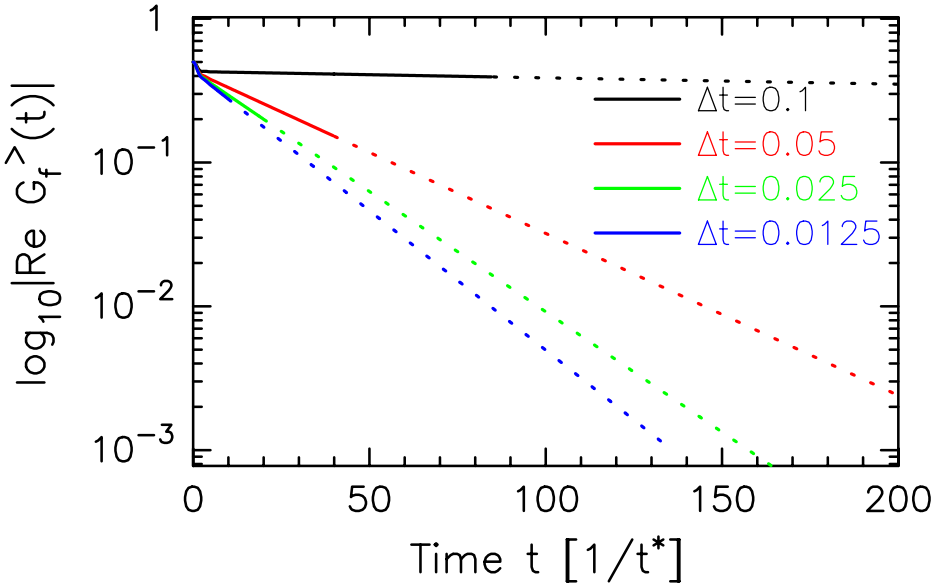
- Exact relations can be computed for the first three moments of the localized electron DOS [with or without an additional Fermi factor $f(\omega)$].
- The Matsubara frequency (imaginary axis) Green's functions can be calculated by an independent procedure, and compared with the results predicted by the DOS through the spectral formula.

Bethe Lattice

Numerical results

U=1 Bethe Lattice (Extrapolation of long-time tails)

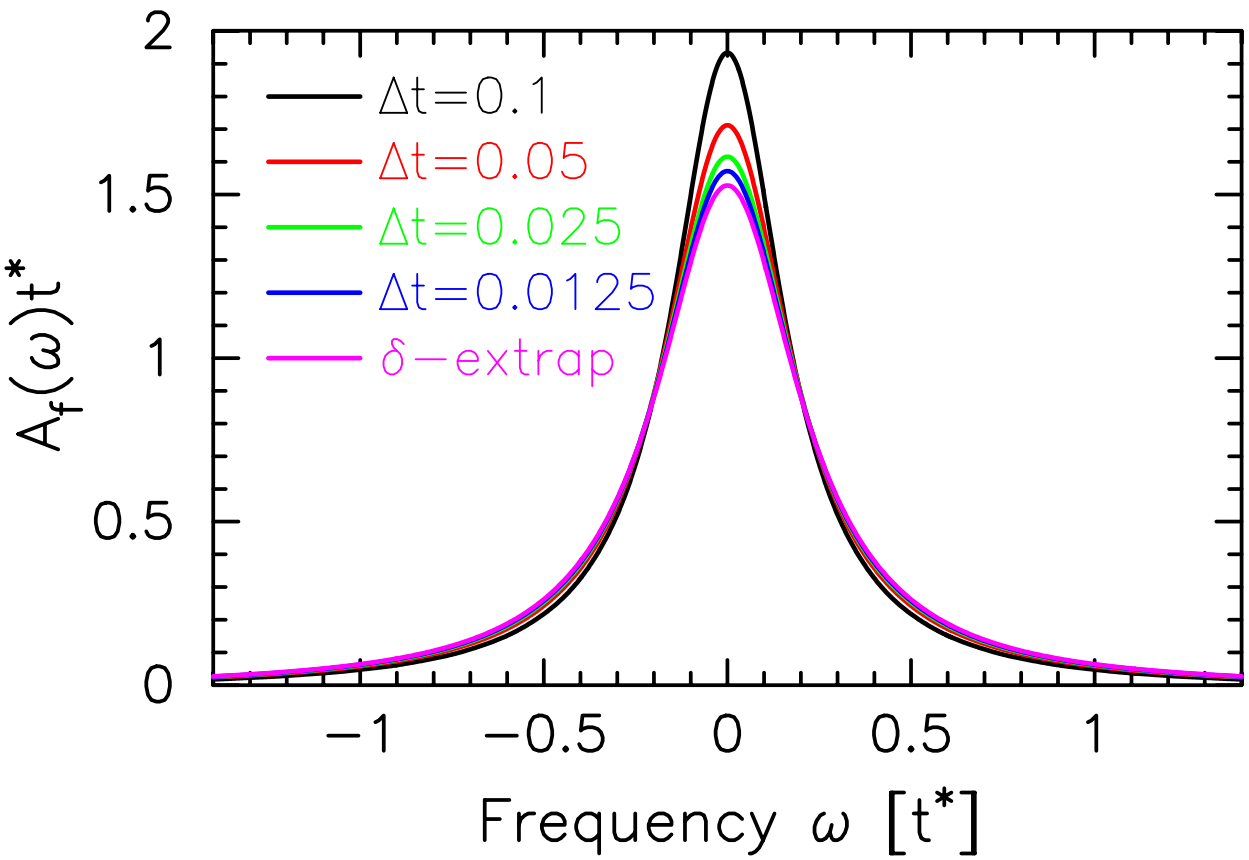




High temperature (T=5)

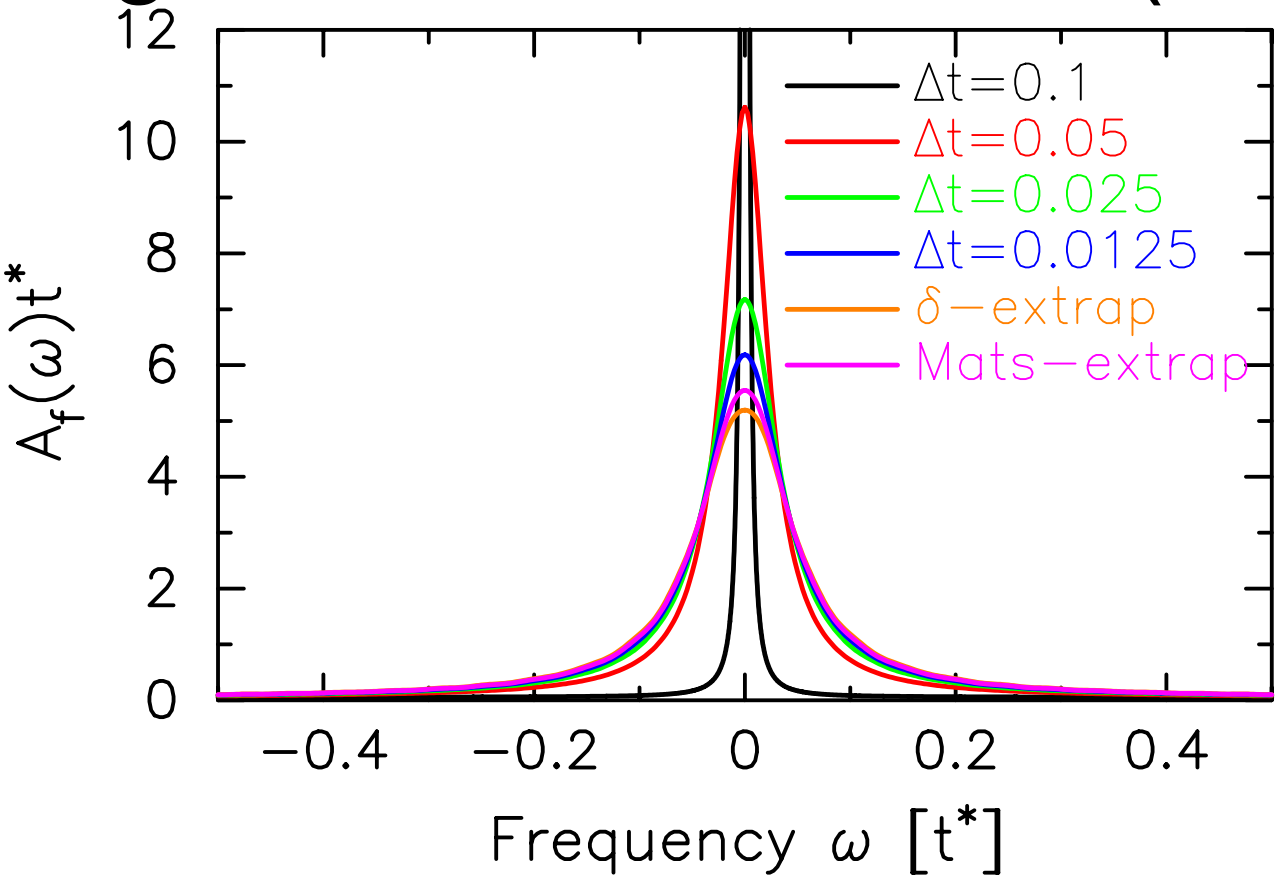
Low temperature (T=0.15)

Scaling of $\Delta t \rightarrow 0$ for T=5 (Bethe)



- We extrapolate the DOS to $\Delta t \rightarrow 0$ by **using a polynomial fit** for each frequency. The extrapolated DOS has an error of **0.1%** for the first moment, **0.03%** for the second moment and **0.003%** for the Matsubara frequency Green's functions.

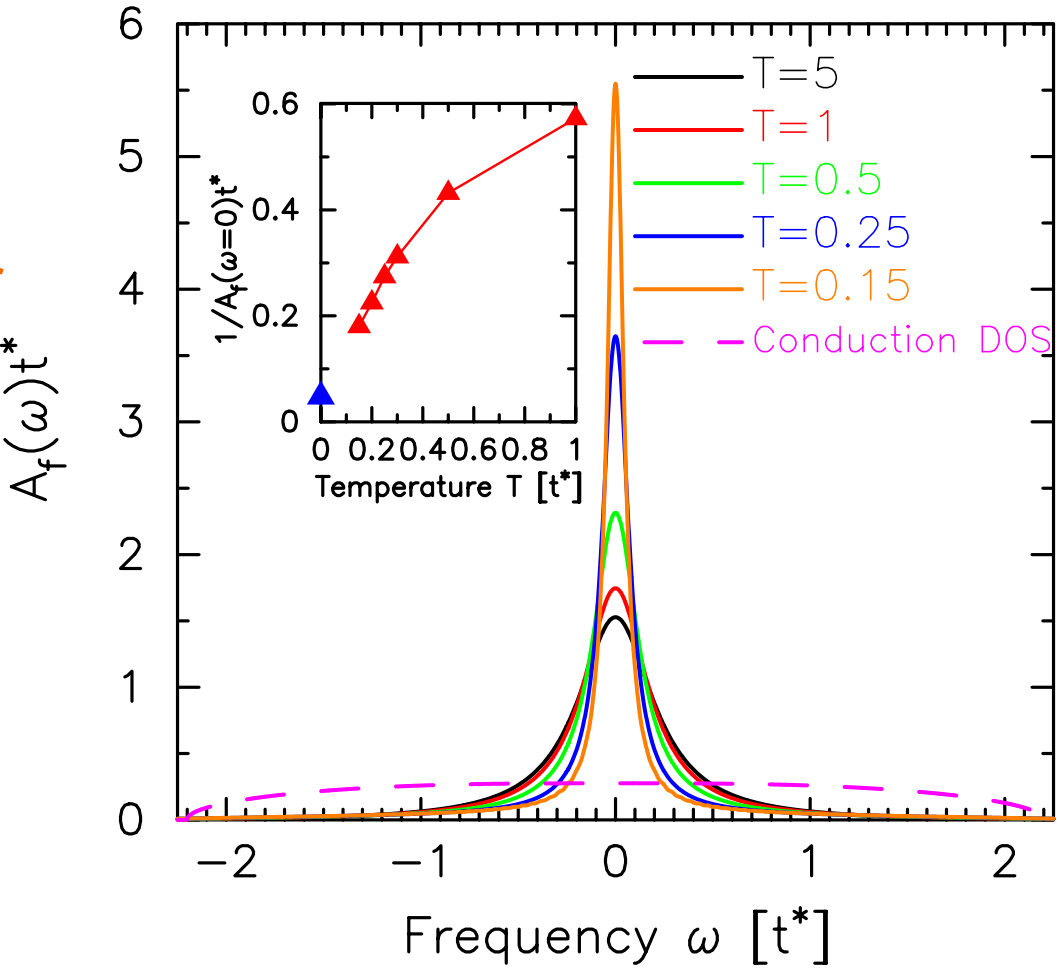
Scaling of $\Delta t \rightarrow 0$ for T=0.15 (Bethe)



- We extrapolate the DOS to $\Delta t \rightarrow 0$ by **forcing the spectral formula for the lowest Matsubara frequency to hold**. The extrapolated DOS has an error of **1%** for the first moment, **1.5%** for the second moment and **0.07%** for the Matsubara frequency Green's functions.

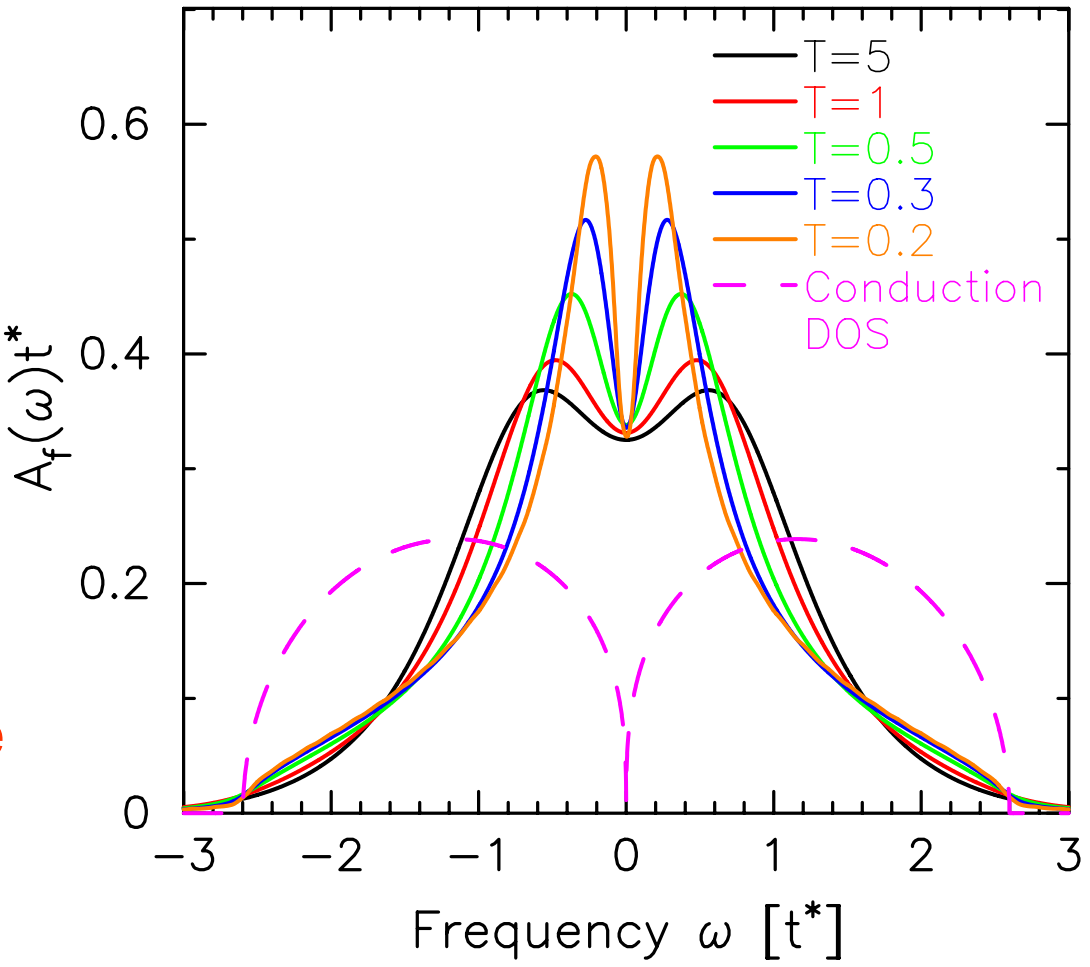
Summary plot for U=1(Bethe)

- The DOS sharpens as T→0, **but it does not sharpen to a delta function**, rather we estimate the peak-height is about 20 at T=0 (see inset).
- Note how **broad** the conduction-electron DOS is in comparison (dashed line).



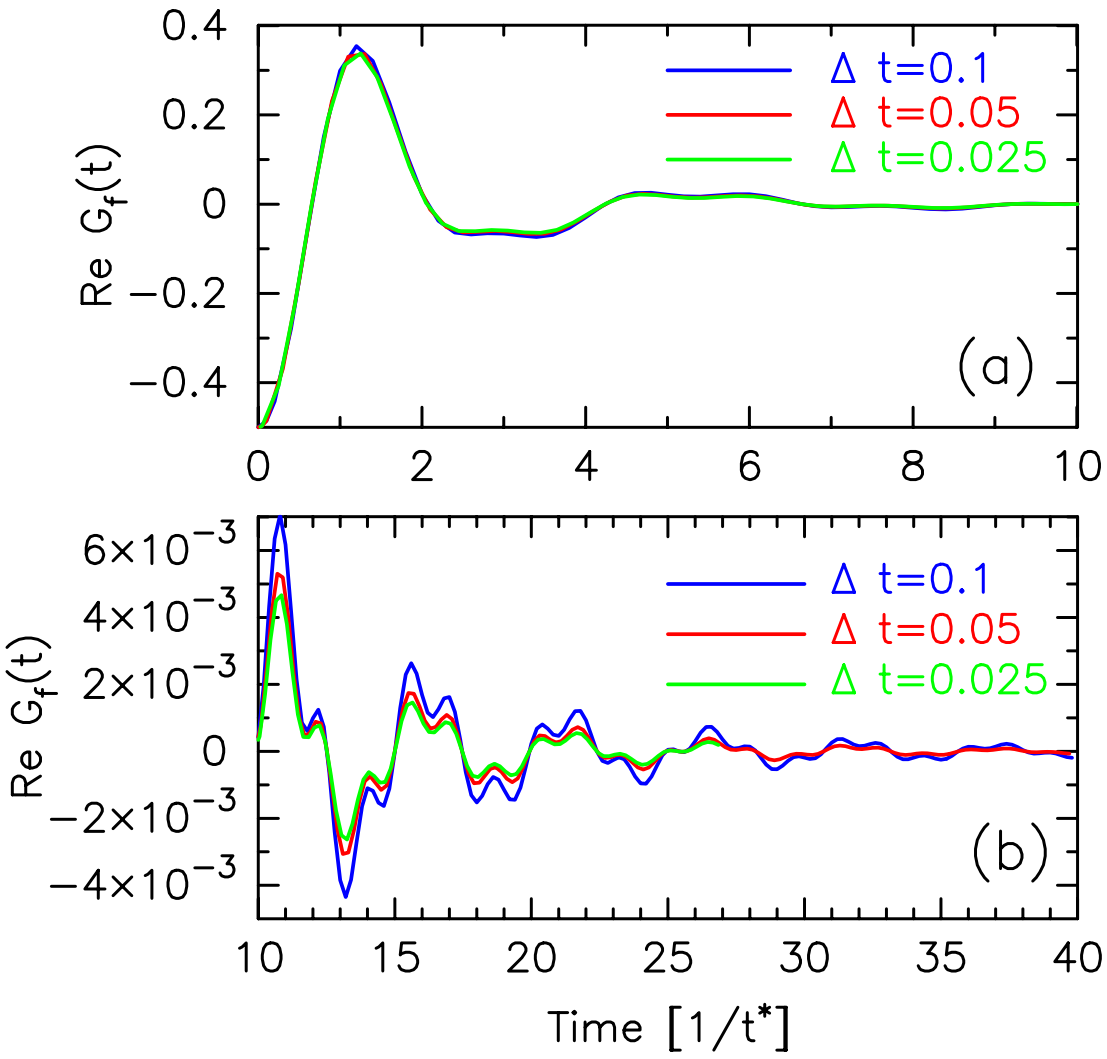
Summary plot for U=2 (Bethe)

- At the critical value of U for the Mott transition, we expect the DOS to have a **pseudogap** at T=0.
- The evolution of the pseudogap is **slow in temperature**, but can be seen in the figure.
- Note how the DOS **"pinches in"**, with the peaks pushing close to the **"gap edge"**.



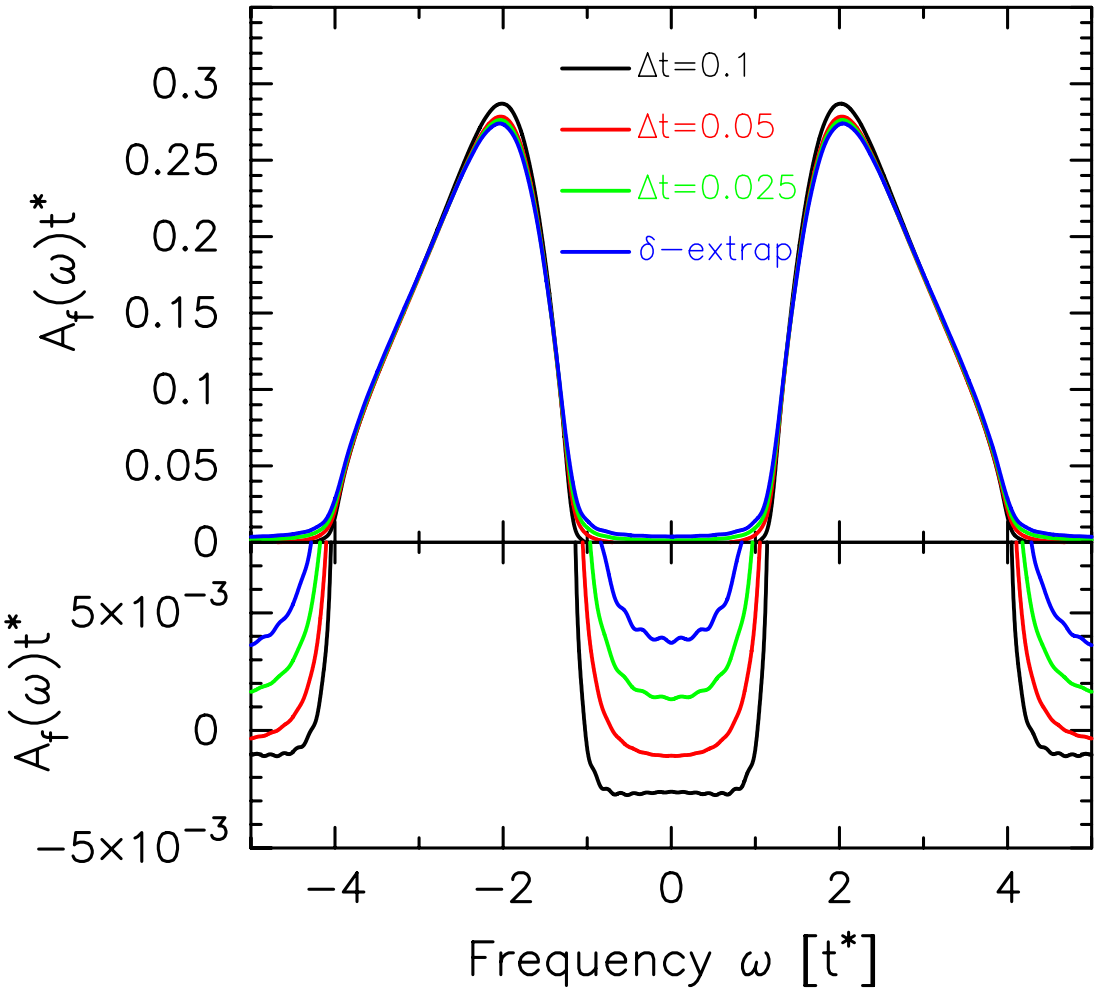
Real-time data for U=5, T=1(Bethe)

- Note the **strong oscillations** that enter at long times, which make it hard to extrapolate the real-time data.
- Surprisingly, the **period of the oscillations appears to be independent of the discretization size**, only the amplitude shrinks as $\Delta t \rightarrow 0$.
- Unfortunately, **a direct extrapolation** to $\Delta t=0$ on the real-time data produces a **poorer quality DOS** than the results at a fixed value of Δt.
- The extrapolation schemes for the real frequency DOS **do not work** in the Mott insulator.



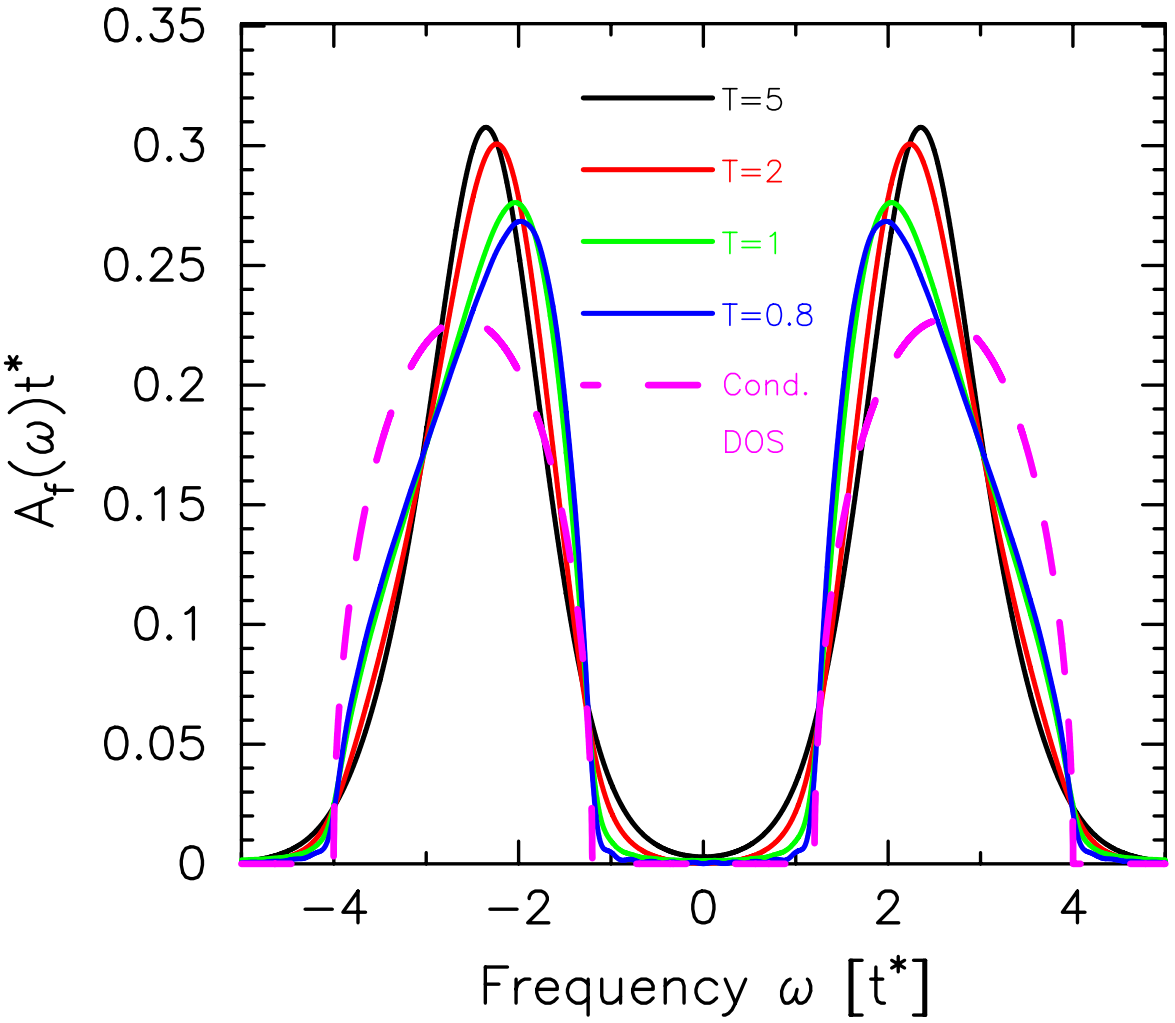
Summary plot for U=5, T=1(Bethe)

- In the Mott insulator, we expect the DOS to have a **gap** at T=0.
- The gap region **fills in with an exponentially small DOS** as T increases.
- Being able to **accurately** determine the DOS in the gap region is **very difficult** because there is **no** extrapolation procedure for large times, and the extrapolations on Δt don't work either.



Summary plot for U=5 (Bethe)

- The gap **clearly is forming** as the temperature is reduced, but we are **severely limited** by how low we can go in temperature and still be able to **accurately** determine the DOS.

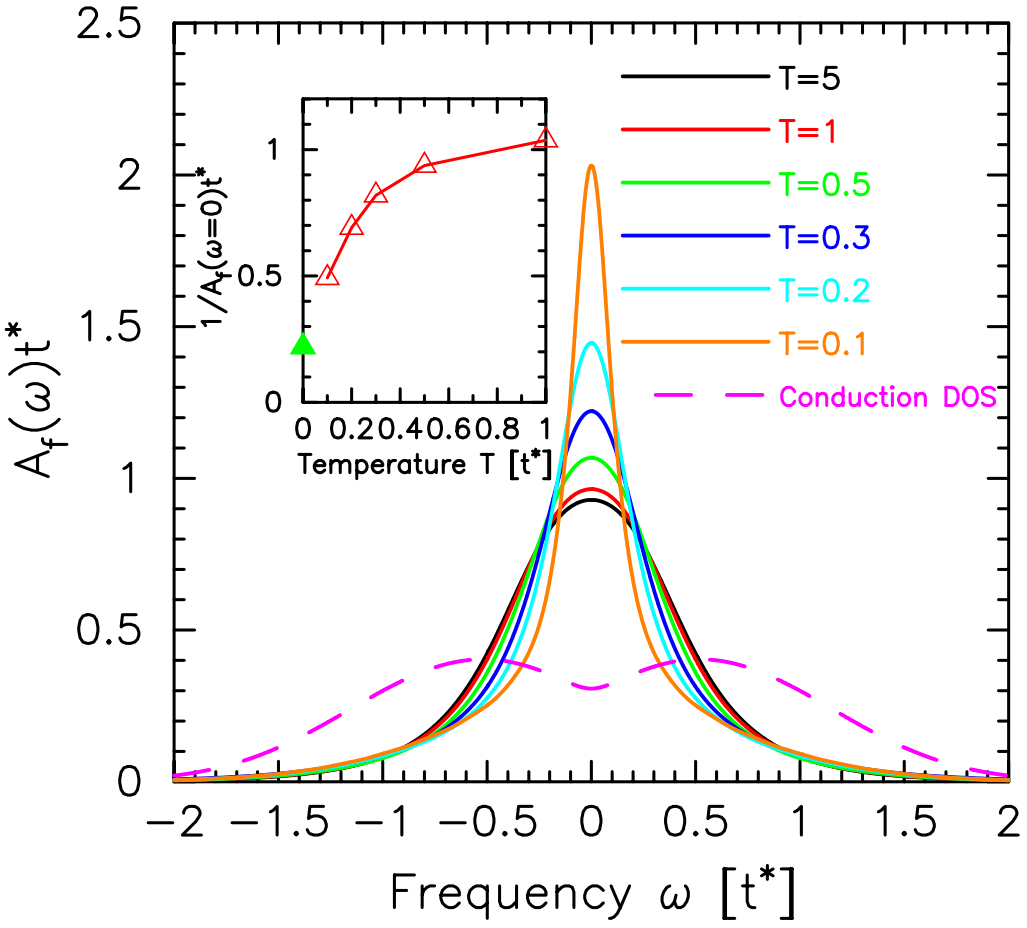


Hypercubic Lattice

Numerical results

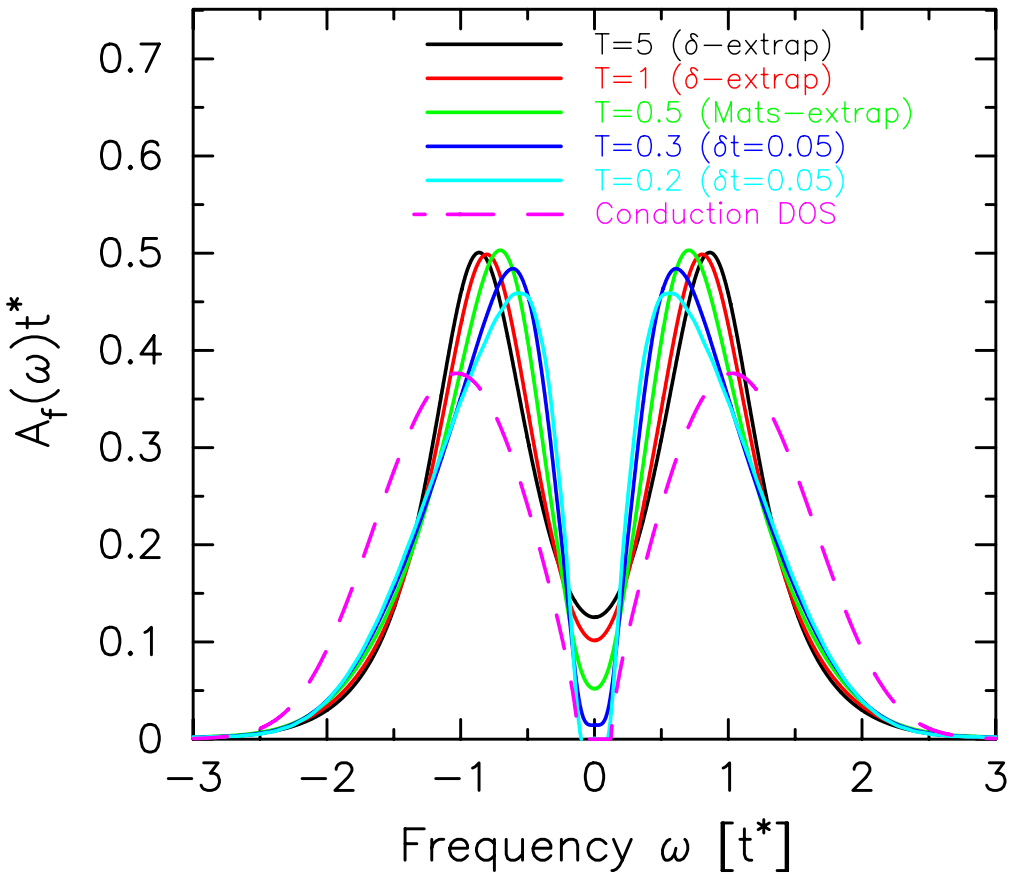
Summary plot for U=1(hc)

- The DOS sharpens as T→0, **but it does not sharpen to a delta function**, rather we estimate the peak-height is about 5 at T=0 (see inset).
- Note how the conduction-electron DOS has a dip at the chemical potential, which is not seen in the f-electron DOS (dashed line).



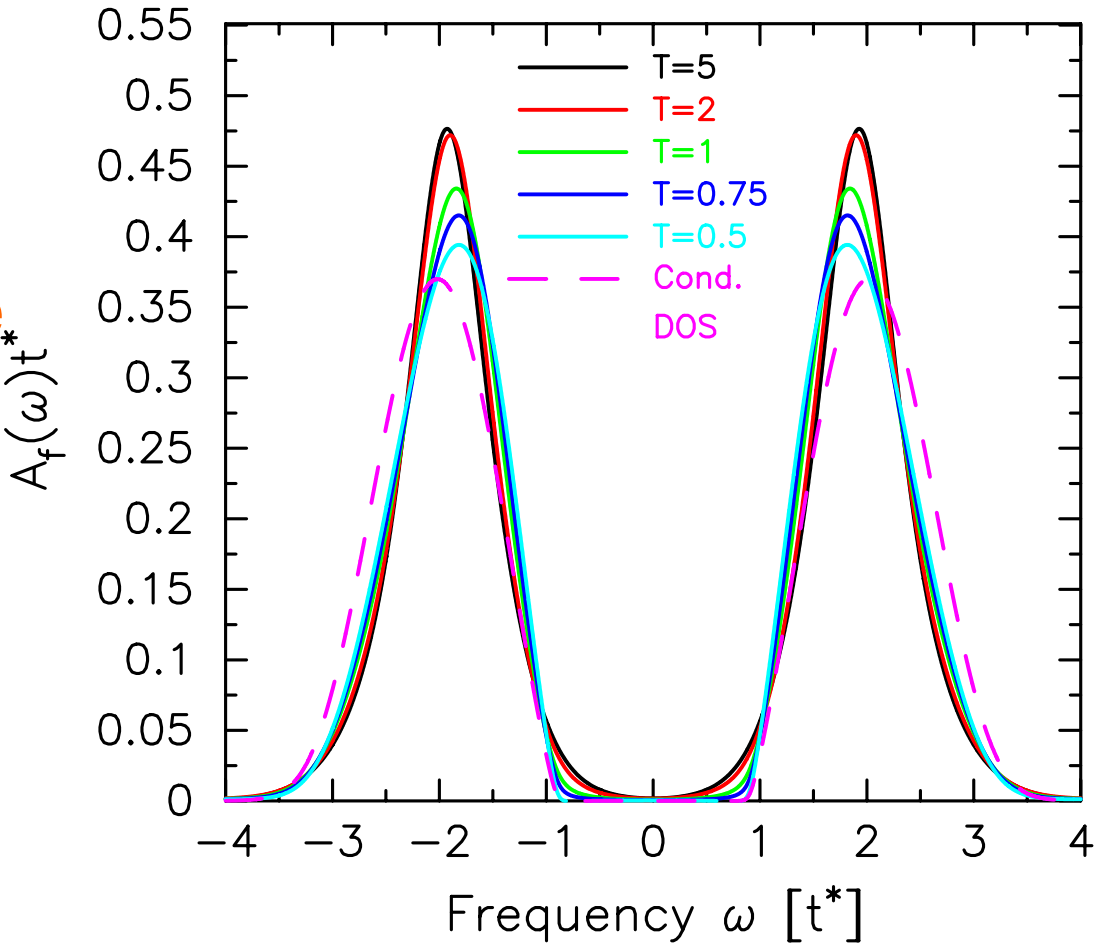
Summary plot for U=1.5 (hc)

- Near the critical value of U for the Mott transition, we expect the DOS to have a **pseudogap** at T=0.
- The evolution of the pseudogap is clear in the figure.
- Note how the DOS **"pinches in"**, with the peaks pushing close to the **"gap edge"**.



Summary plot for U=4 (hc)

- The "gap" **clearly is forming** as the temperature is reduced. Here we can go farther down in temperature and still **accurately** determine the DOS.



Conclusions

- Showed how to implement an **efficient parallel algorithm** to solve the **Keldysh problem** for strongly correlated electrons described by the Falicov-Kimball model.
- The procedure was applied to the **simplest problem**---the localized electron spectral function. This problem is a useful test case because one can examine the accuracy in great detail and understand systematics related to approximating continuous matrix operators by discrete approximants.

Future work

- Generalize this approach to solve for the **nonlinear**, **nonequilibrium** response of the conduction electrons in a strong electromagnetic field.
- Apply the nonequilibrium formalism to **nanostructure transport** and investigate both **electrical** and **thermal** transport within a **self-consistent framework**.