

# Parallelizing the Keldysh formalism for strongly correlated electrons

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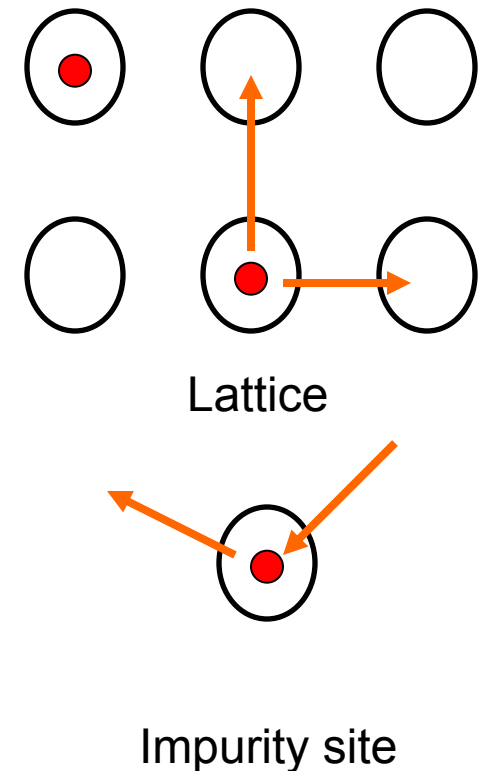
Thanks to Volodmyr Turkowski and Veljko Zlatic' for collaborating on this work.

# Military Relevance

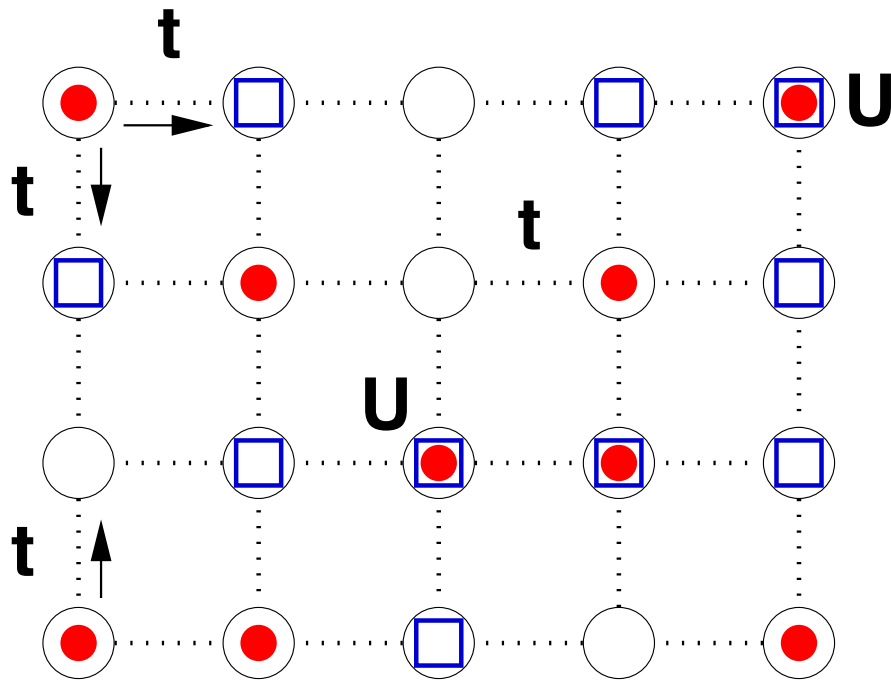
- Strongly correlated electron materials have properties (conductivity, magnetism, superconductivity) that can be **tuned** by varying pressure, temperature, or doping.
- They have potential for use in so-called **smart materials technologies**.
- Materials like plutonium have strong electron correlations, which may play a role in **nuclear stockpile stewardship**.
- Many military applications involve subjecting materials and devices to **strong electromagnetic fields**, where **nonequilibrium** and **nonlinear** effects are important.

# 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**.



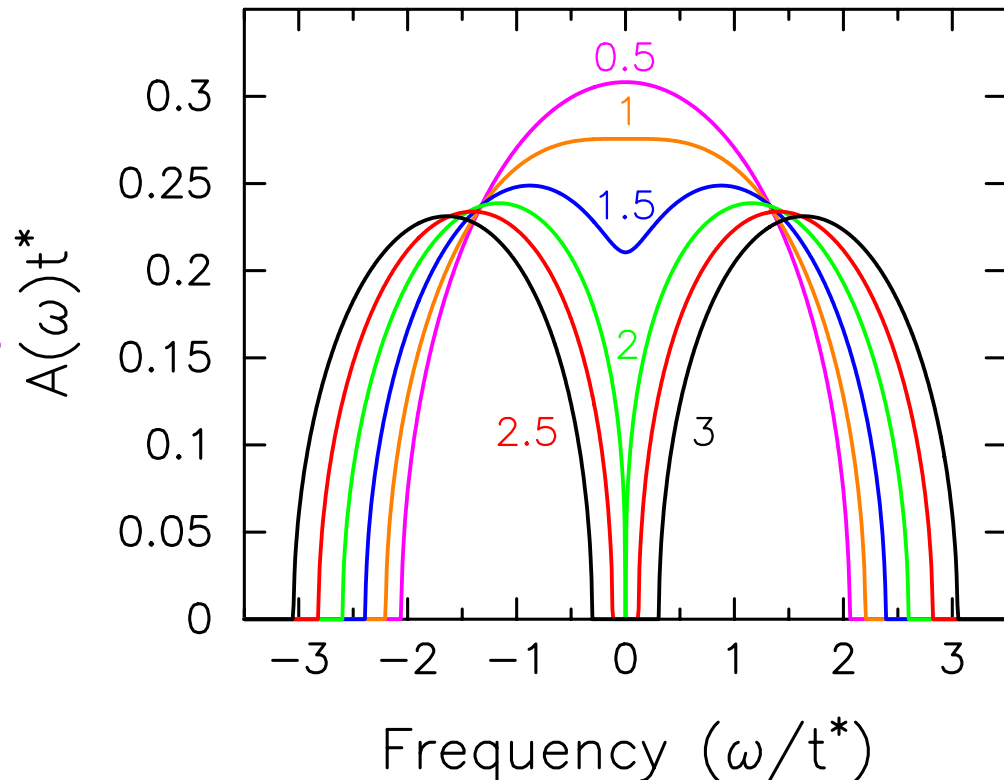
# Falicov-Kimball Model



- 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)

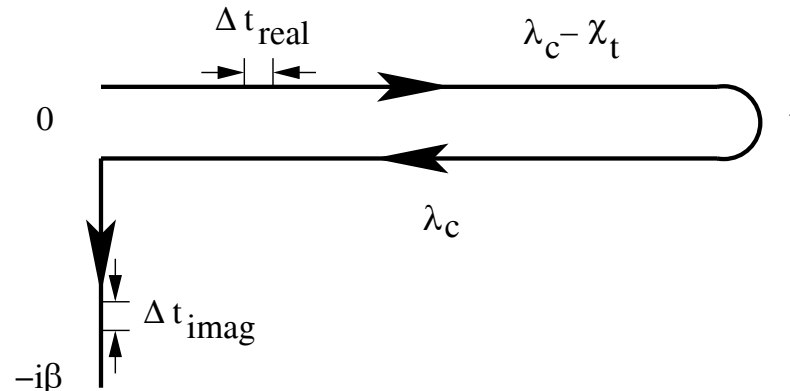
- The Falicov-Kimball model is **not** a Fermi liquid.
- On a Bethe lattice, it has a **Mott transition** at  $U=2$  and half filling.
- The conduction-electron DOS is **independent of temperature**, and **continuously decreases to zero** at the chemical potential as  $U$  increases. Then a **true gap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



# DOS (localized electrons)

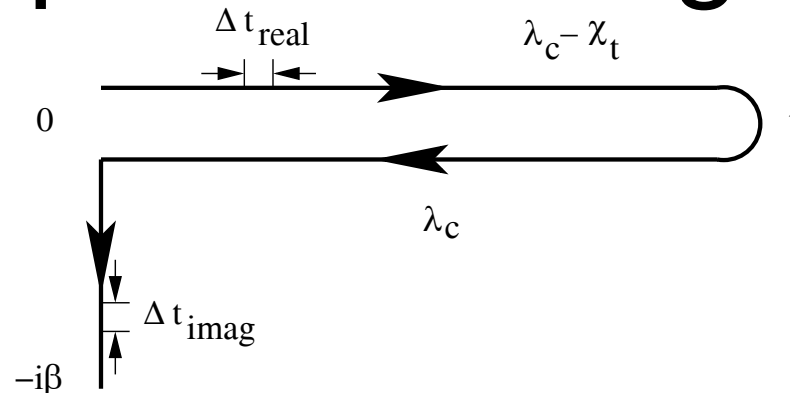
- The localized electrons **interact** with the conduction electrons when they sit on the same lattice site.
- Since the hopping of the conduction electrons on the lattice is mimicked by a time-dependent field (called  $\lambda$ ) for the impurity, the localized electrons **feel an additional time-dependent field** (called  $\chi$ ) 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 **Keldysh 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 Keldysh 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  $\lambda$ , the interaction strength  $U$ , and the temperature, **this procedure is easily parallelized**.



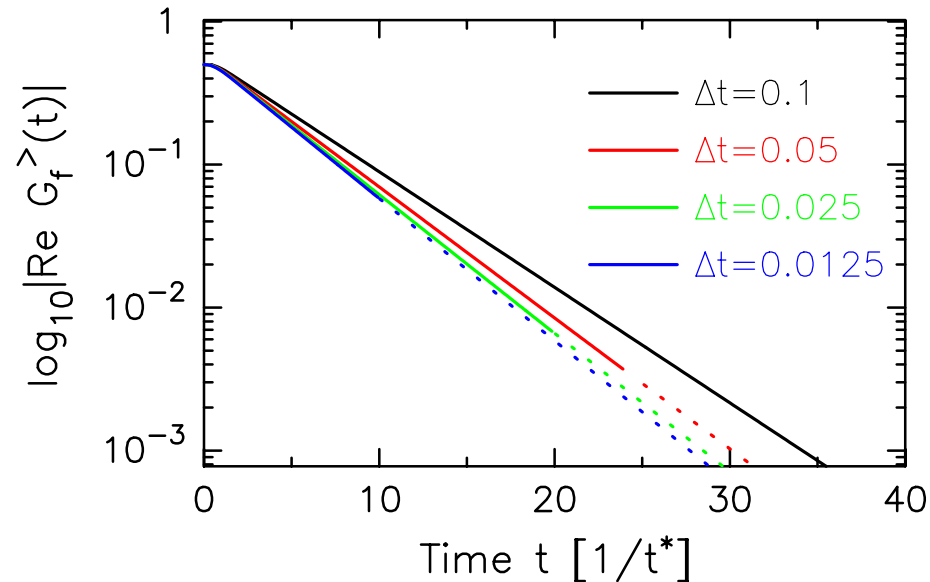
# Parallel implementation

- (1) **Solve** for the conduction electron Green's function to determine the **dynamical mean field**  $\lambda$  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.

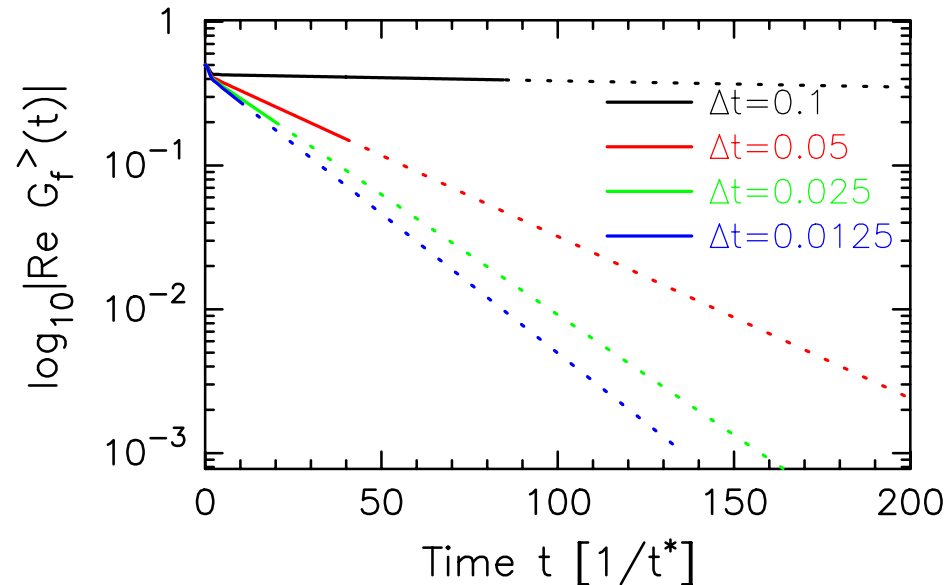
# Numerical issues

- 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.**

# U=1 (Extrapolation of long-time tails)



High temperature ( $T=5$ )

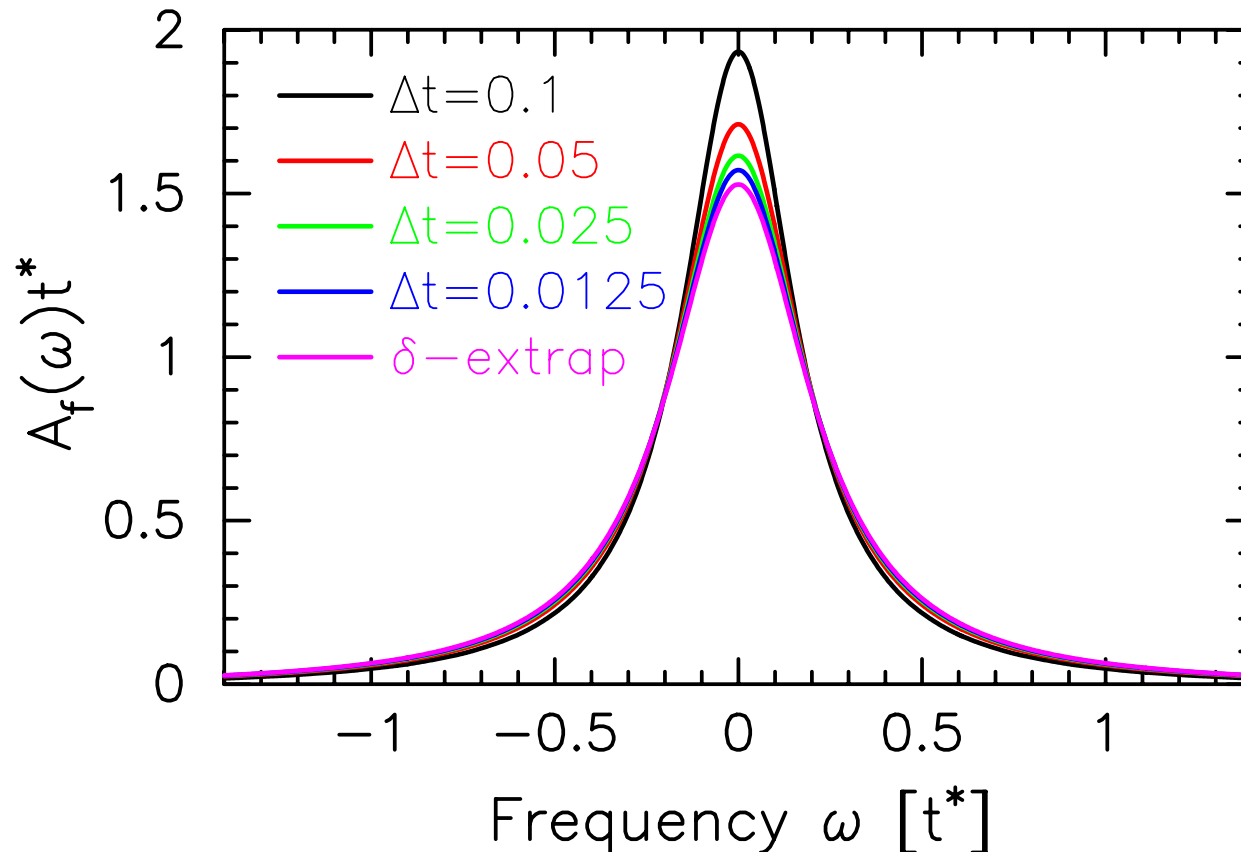


Low temperature ( $T=0.15$ )

# Sum rules

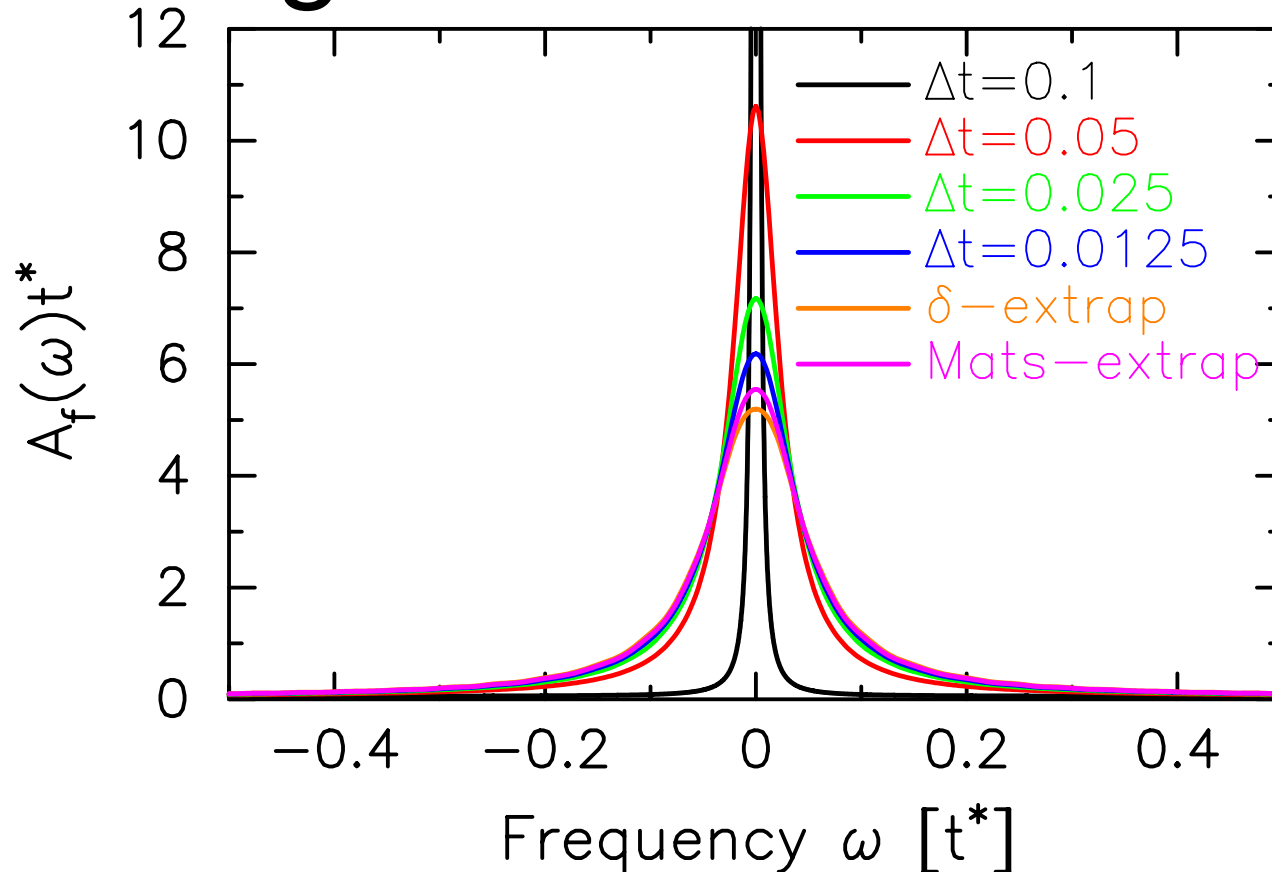
- Exact relations can be computed for the first three moments of the localized electron DOS [with or without an additional Fermi factor  $f(\omega)$ ].
- The Matsubara frequency (imaginary axis) Green's functions can be calculated by an independent procedure, and compared with the results predicted by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

# Scaling of $\Delta t \rightarrow 0$ for $T=5$



- 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.

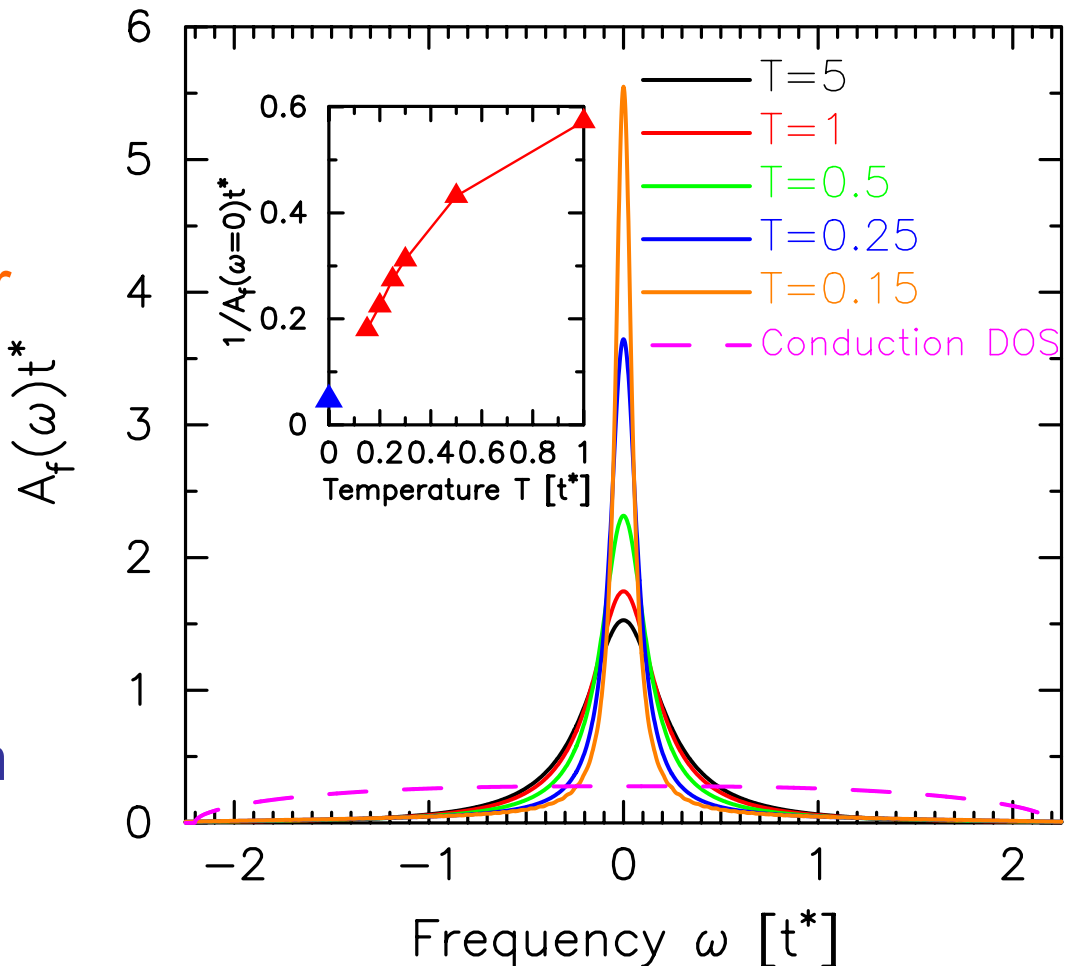
# Scaling of $\Delta t \rightarrow 0$ for $T=0.15$



- 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.

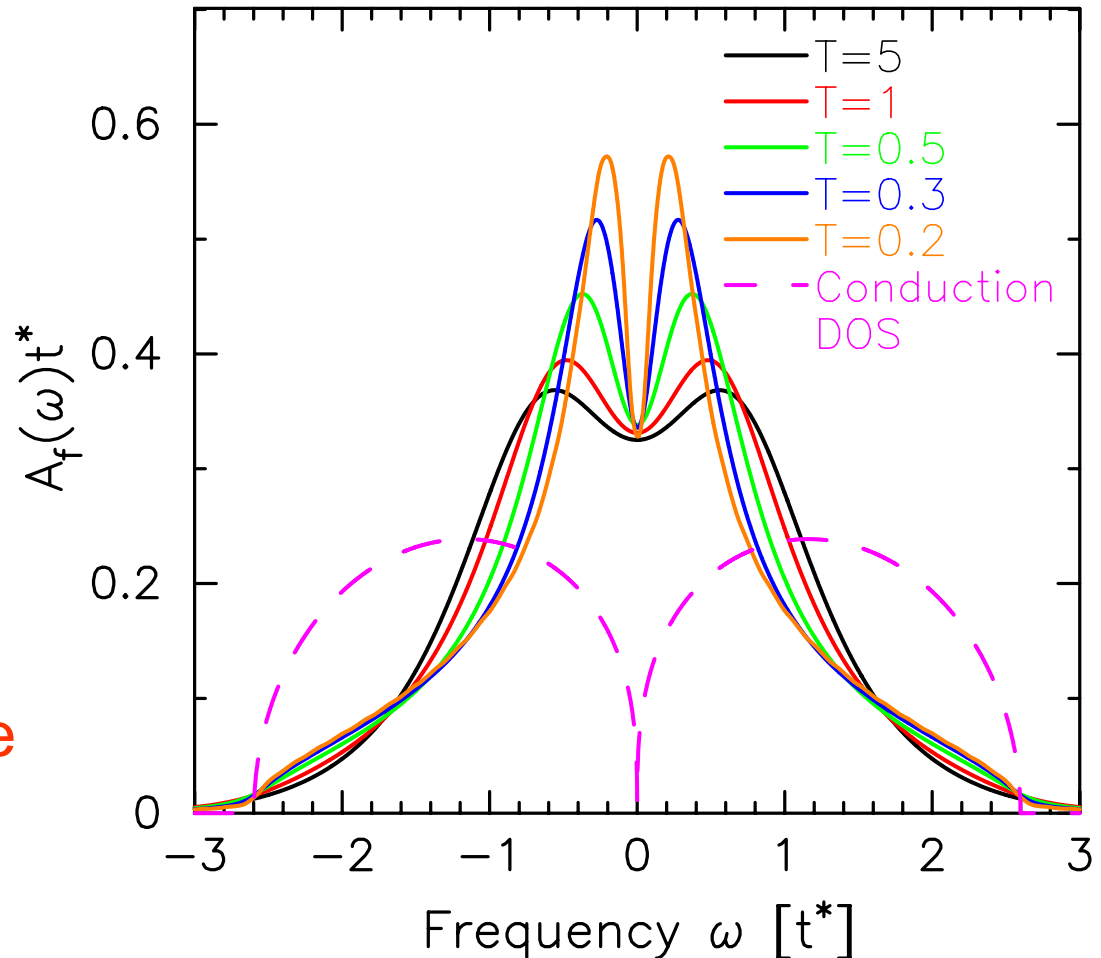
# Summary plot for $U=1$

- The DOS sharpens as  $T \rightarrow 0$ , **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 $U=2$

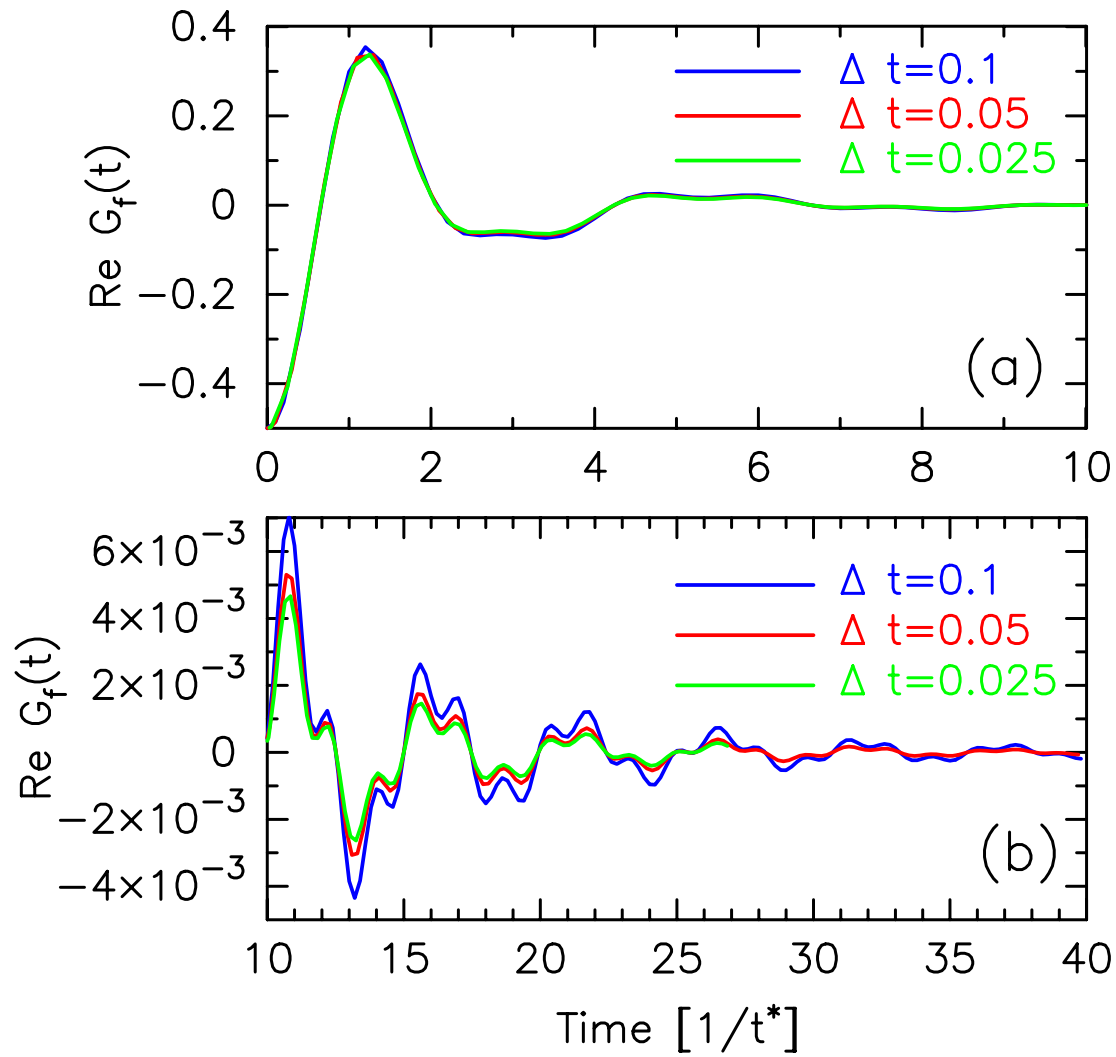
- At the critical value of  $U$  for the Mott transition, we expect the DOS to have a **pseudogap** at  $T=0$ .
- The evolution of the pseudogap is **slow in temperature**, but can be seen in the figure.
- Note how the DOS “**pinches in**”, with the peaks pushing close to the “**gap edge**”.





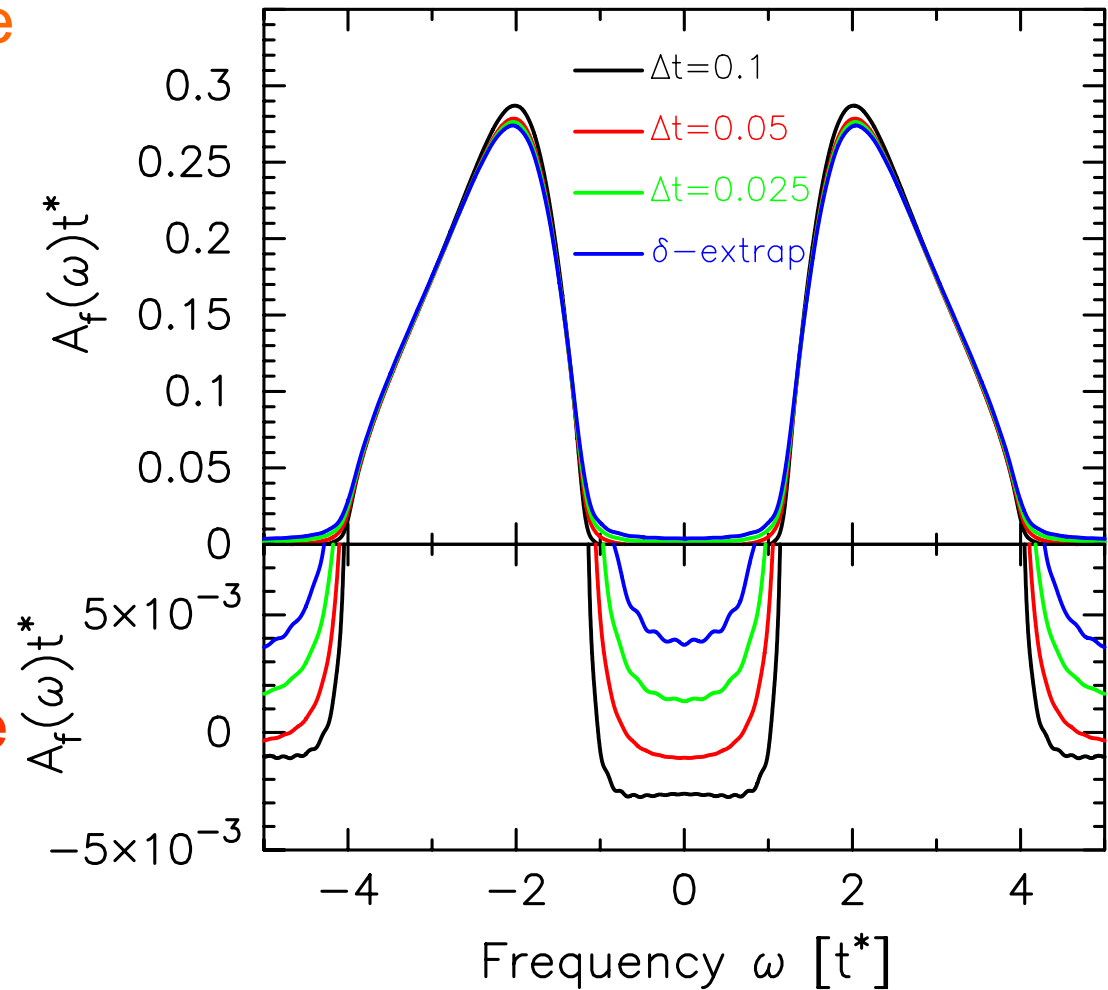
# Real-time data for $U=5$ , $T=1$

- 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  $\Delta t$ .
- The extrapolation schemes for the real frequency DOS **do not work** in the Mott insulator.



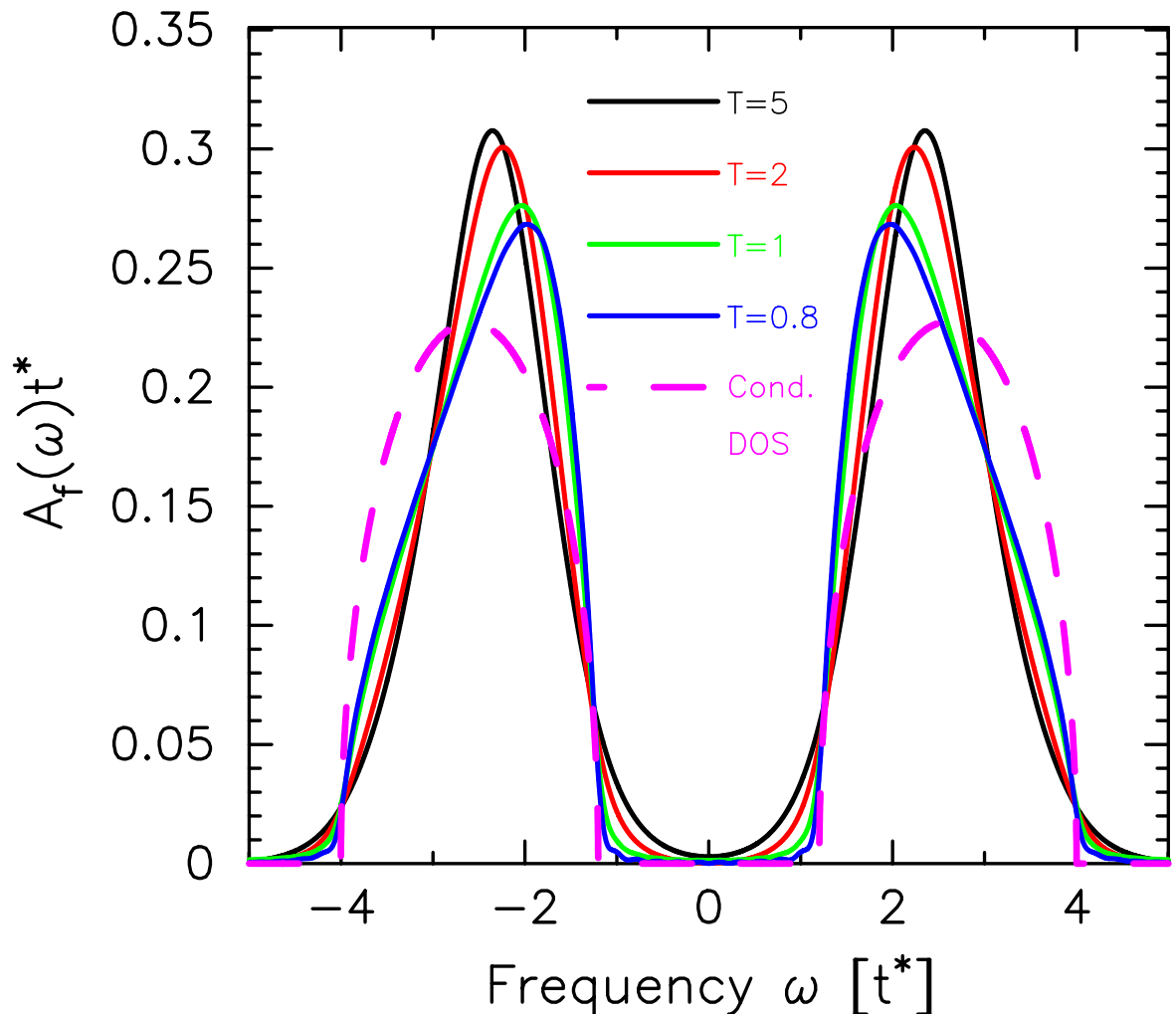
# Summary plot for $U=5$ , $T=1$

- 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  $\Delta t$  don't work either.



# Summary plot for $U=5$

- 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.



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