DMFT and two-particle correlations

ERIK VAN LOON, LUND UNIVERSITY, JUNE 24TH 2021

Electronic correlations

- Electrons are charged particles, their motion is not independent
- Coulomb interaction responsible for several interesting effects in condensed matter physics
  - Excitons in semiconductors
  - Plasmons in the electron gas
  - Magnetism (Stoner, Heisenberg)
  - Fermi liquid theory
  - **Mott metal-insulator transition** 

Purpose of this talk

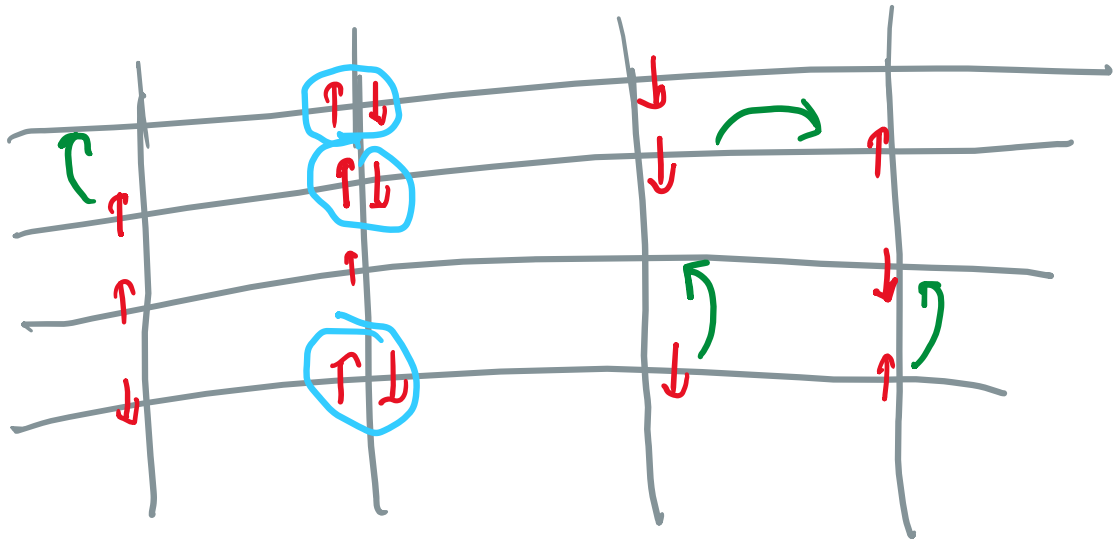
- Dynamical mean-field theory is a standard theoretical/computational approach for correlated electron systems.
- Dynamical mean-field theory can be a complicated thing, with many computational subtleties.
- Here, simple one-orbital systems at particle-hole symmetry, everything is relatively simple and the structure becomes clear.
- Modern DMFT is ready to address questions about two-particle correlations.

This talk

- Mainly about the paper:
  EvL, Friedrich Krien and Andrey Katanin, Phys. Rev. Lett. **125**, 136402 (2020)
- Relating the DMFT metal-insulator transition to known concepts of statistical physics of phase transitions

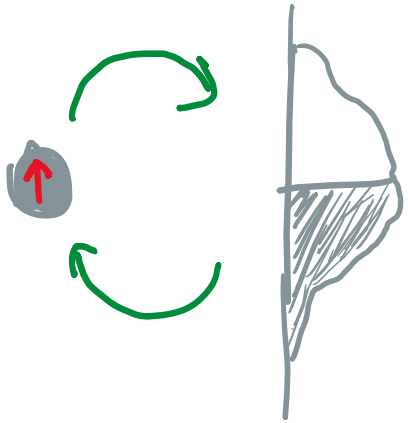
- Simultaneous activity at TU Wien (Toschi group)

Hubbard model



$$\hat{H} = -\sum_{\substack{ij \\ \sigma=\uparrow,\downarrow}} t_{ij}\, c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

Dynamical Mean-Field Theory



Dynamical: The likelihood of leaving the site and coming back at a later time depends on the time difference, i.e., on the frequency.

Mott metal-insulator transition: takes place at energies close to the Fermi level, that determines if a system is a metal or an insulator.

Review: Georges et al., 1996, Rev. Mod Phys

Two-particle level

- If there is an ↑ electron on a site at time t_1,
  what is the probability to find an ↑/↓ there at time t_2?
- If a field is applied, how does the system respond?
  - Linear response
  - Static field ($\omega = 0$) or not?

$$\frac{d}{d\mu}\left(\dots e^{-\beta H}\right)\curvearrowright$$

- Mean-field theory is a self-consistent theory, how is the convergence?

Reminder: Ising model & MFT

$$H = -J \sum_{\langle ij \rangle} S_i^z \cdot S_j^z - \sum_i h S_i^z$$

$$\Downarrow$$

$$H^{imp} = -(h + h^{MF}) S^z$$

&

$$h^{MF} = J z m$$

$$m = \langle S^z \rangle^{imp}$$

Solver

$$= \tanh(\beta(h + h^{MF}))$$

Lattice only here!

Reminder: Weiss mean-field theory

- Response to a change in the external magnetic field $\chi = \frac{dm}{dh}$
- $\chi^{imp} = \frac{dm^{imp}}{dh}$
- But that is not everything!
  - χ^{imp} is the response while $h^{MF} = Jzm$ is held fixed
  - To calculate χ, we need to take into account change in h^{MF} as well
  - $\chi = \frac{dm}{dh} = \frac{dm^{imp}}{dh} + \frac{dm^{imp}}{dh^{MF}}\frac{dh^{MF}}{dh} = \chi^{imp} + \chi^{imp} Jz \frac{dm}{dh}$
  - $\chi = \chi^{imp}/(1 - Jz\,\chi^{imp})$
- Qualitatively important, χ^{imp} is divergence free, χ not → Phase transition due to denominator

DMFT: how it works in one slide

$$H = -\sum_k t_k \, c_k^\dagger c_k + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

to

$$S^{imp} = \sum_\nu (\Delta_\nu - i\nu)\, c_\nu^\dagger c_\nu + U \int d\tau \, n_\uparrow(\tau) n_\downarrow(\tau)$$

Δ_ν = vector

&

$$\sum_k \frac{1}{g_\nu^{-1} + \Delta_\nu - t_k} \equiv g_\nu \quad \text{(self-consistency)}$$

↑ lattice only here

where $g_\nu = -\langle c c^\dagger \rangle_\nu^{imp}$ is AN expectation vALue of S^{imp}

$$\frac{\partial g_m}{\partial \Delta_n} \neq 0$$

Density and response

- Self-consistency condition implies $n^{imp} = n$. $\sim \langle S^z \rangle$ in Weiss theory
- What if I change the chemical potential?
- $n^{imp}(\mu, \Delta)$ and Δ is determined self-consistently, i.e., Δ depends on μ.
- $g(i\nu_m)$ depends on $\Delta(i\nu_n)$, also for $m \neq n$.
- Response function is a matrix equation in frequency.

$$\frac{\partial n^{imp}}{\partial \mu} + \sum_m \frac{\partial n^{imp}}{\partial \Delta_m} \frac{\partial \Delta_m}{\partial \mu}$$

DMFT response: nonlocal correction

- The corrections to χ^{imp} are due to the embedding of the atom into the lattice, i.e., the fact that there are other sites.
- In the formula below, $\tilde{G}_{\boldsymbol{k}} = G_{\boldsymbol{k}} - \sum_{\boldsymbol{k}} G_{\boldsymbol{k}}$, or $\tilde{G}_{ij} = G_{ij} - \delta_{ij} G_{ii}$

$$X_{\mathbf{q}=0,\omega=0} = -\frac{d\langle n\rangle}{d\mu} = -\frac{\partial\langle n\rangle^{\mathrm{imp}}}{\partial\mu} - \sum_{\nu\sigma} \frac{\partial\langle n\rangle^{\mathrm{imp}}}{\partial\Delta_{\nu\sigma}} \frac{\partial\Delta_{\nu\sigma}}{\partial\mu}$$

$$= \chi_{\omega=0} + \sum_{\nu\nu'\sigma\sigma'} \chi_{\omega=0}\lambda_{\nu\sigma,\omega=0} \sum_{\mathbf{k}} \tilde{G}^2_{\nu\sigma\mathbf{k}} \left[\gamma_{\nu\nu\sigma\sigma,\omega=0} \sum_{\mathbf{k}} \tilde{G}^2_{\nu\sigma\mathbf{k}} + \delta_{\nu\nu'}\delta_{\sigma\sigma'} \right]^{-1} \lambda_{\nu'\sigma',\omega=0}\chi_{\omega=0}.$$

EvL, Hafermann, Lichtenstein, Katsnelson
Phys. Rev. B **92**, 085106 (2015)

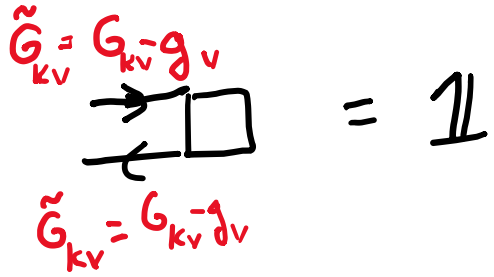
DMFT response: stability

$$\left[\gamma_{\nu\nu\sigma\sigma,\omega=0}\sum_{\mathbf{k}}\tilde{G}^{2}_{\nu\sigma\mathbf{k}}+\delta_{\nu\nu'}\delta_{\sigma\sigma'}\right]^{-1}$$

∂z

- This might diverge! Thermodynamic instability.
- Entirely due to non-local feedback in the DMFT.

$\frac{d_n}{d_\mu} = \infty$ phase separation



$= \mathbb{1}$

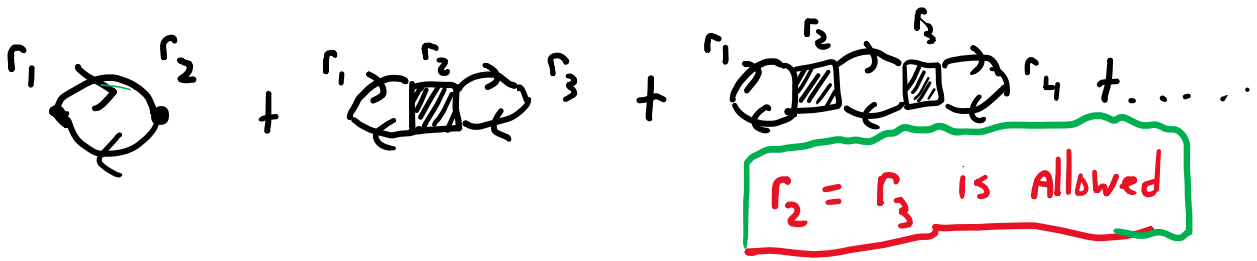
$\tilde{G}$ non-local propagation of electrons

$$\tilde{G}_{ij} = \begin{cases} G_{ij} & i \neq j \\ 0 & i = j \end{cases}$$

DMFT response

- The previous formulas are not how it is usually done!

- Usually approach starts from indepent propagation of two electrons (“bubble”) and adds vertex corrections



Can have entirely local divergences, as discussed by A. Toschi in a previous seminar

Review: Georges et al., 1996, Rev. Mod Phys

Self-consistency & Jacobian

- $\Delta(i\nu_n) = f[\Delta(i\nu_m)]$
- The eigenvalues of the Jacobian determine how the iterations go, all absolute eigenvalues smaller than 1 implies convergence.
- It is actually possible to analytically calculate the Jacobian and express it in terms of
  - expectation values of the impurity model,
  - and parameters of the lattice Hamiltonian.

See also: H. Strand et al., Phys. Rev. B **83**, 205136 (2011)

Calculating the Jacobian

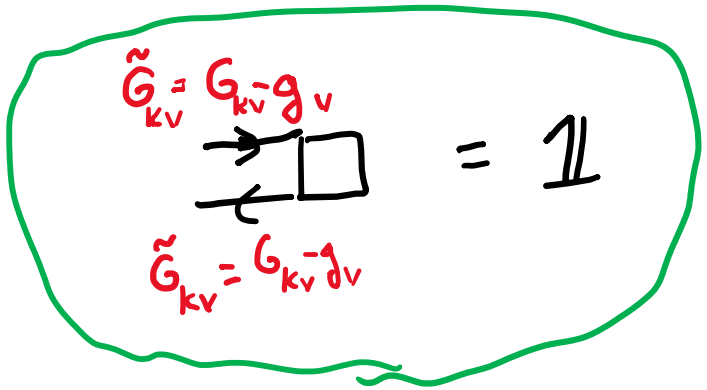
- Jacobian $\frac{\partial \Delta^{\text{new}}}{\partial \Delta^{\text{old}}}$.

$\Delta^{old} \rightarrow g$

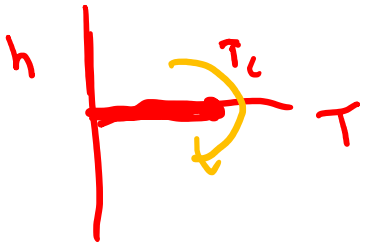
- Non-trivial: $g(i\nu_n)$ depends on $\Delta(i\nu_m)$, matrix equation in frequency.
- $\frac{\partial g(i\nu_n)}{\partial \Delta(i\nu_m)}$ is a two-particle correlation function of the impurity model.

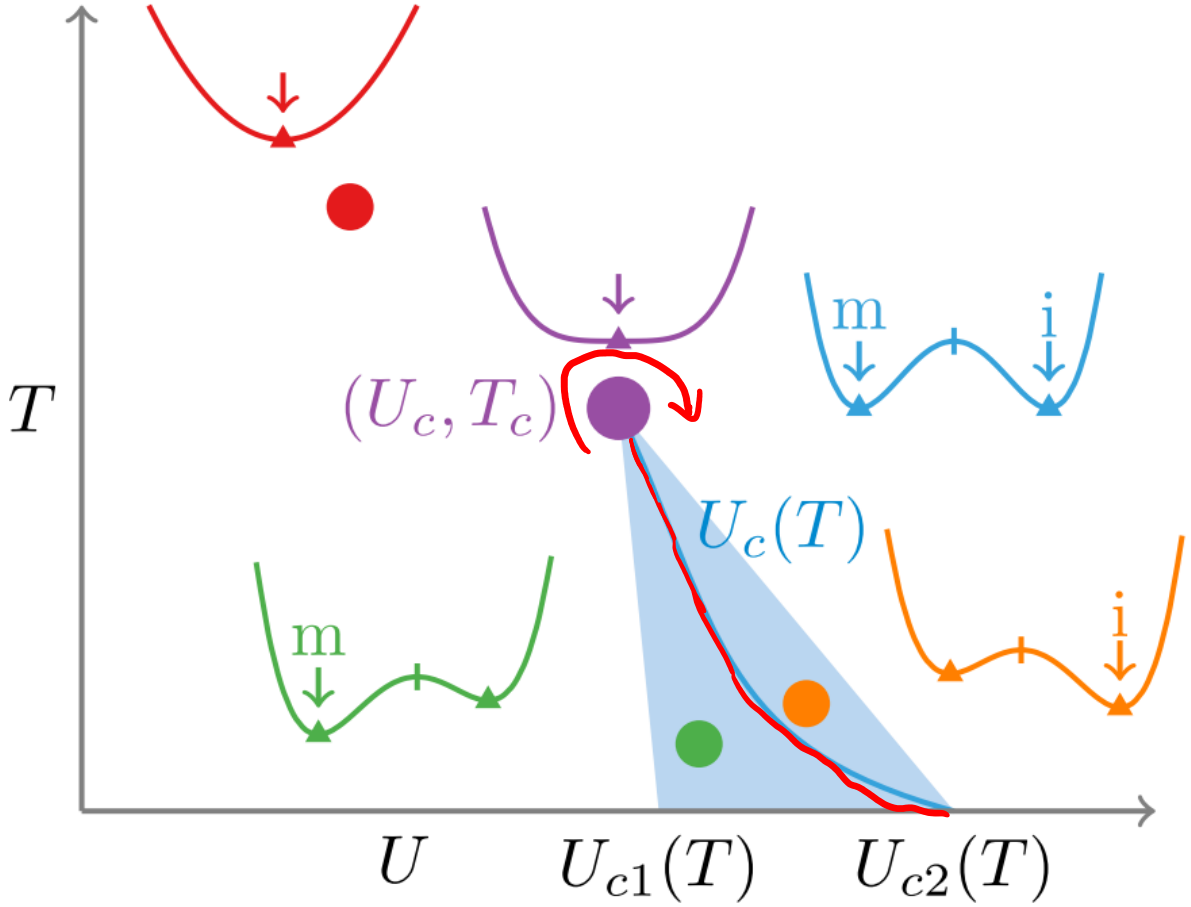
↳ expectation value

- After some calculus… The same equation as before!

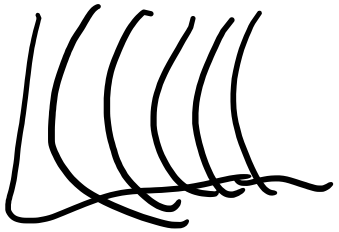


Landau free energy (sketch)





$\frac{\partial^2 \Omega}{\partial x^2} > 0?$



$\frac{\partial g_m}{\partial \Delta_n}$

$\sim g_\Delta$

leading eigenvalue of γ

Landau free Energy & DMFT

- What is the order parameter x?
- What is Ω?

- $\Omega[\Delta] = \Omega_{imp}[\Delta] - \Omega'[\Delta]$
- By definition, $\frac{\delta\Omega}{\delta\Delta} = 0$ at the DMFT self-consistent solution, this fixes $\Omega'[\Delta]$ and we can calculate the Hessian matrix $\delta^2\Omega/\delta\Delta^2$

SC condition

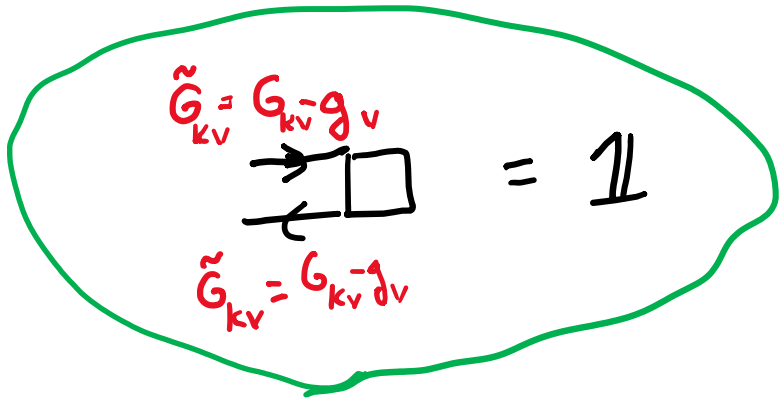
$\frac{\delta^2\Omega}{\partial\Delta_n \partial\Delta_m}$

All eigen values > 0 < 0 $= 0$

- The answer won't surprise you…

Hessian of the Free Energy

- Second-derivative is a matrix equation in frequency
- The sign of $\delta^2\Omega/\delta\Delta^2$ is determined by the same kernel that we have seen several times. Sign changes when

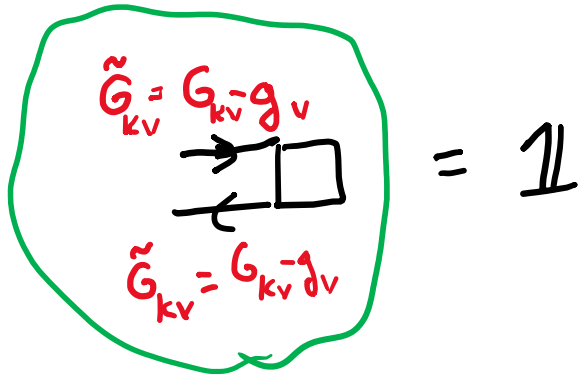


Three times the same matrix

$\frac{dn}{d\mu}$

χ

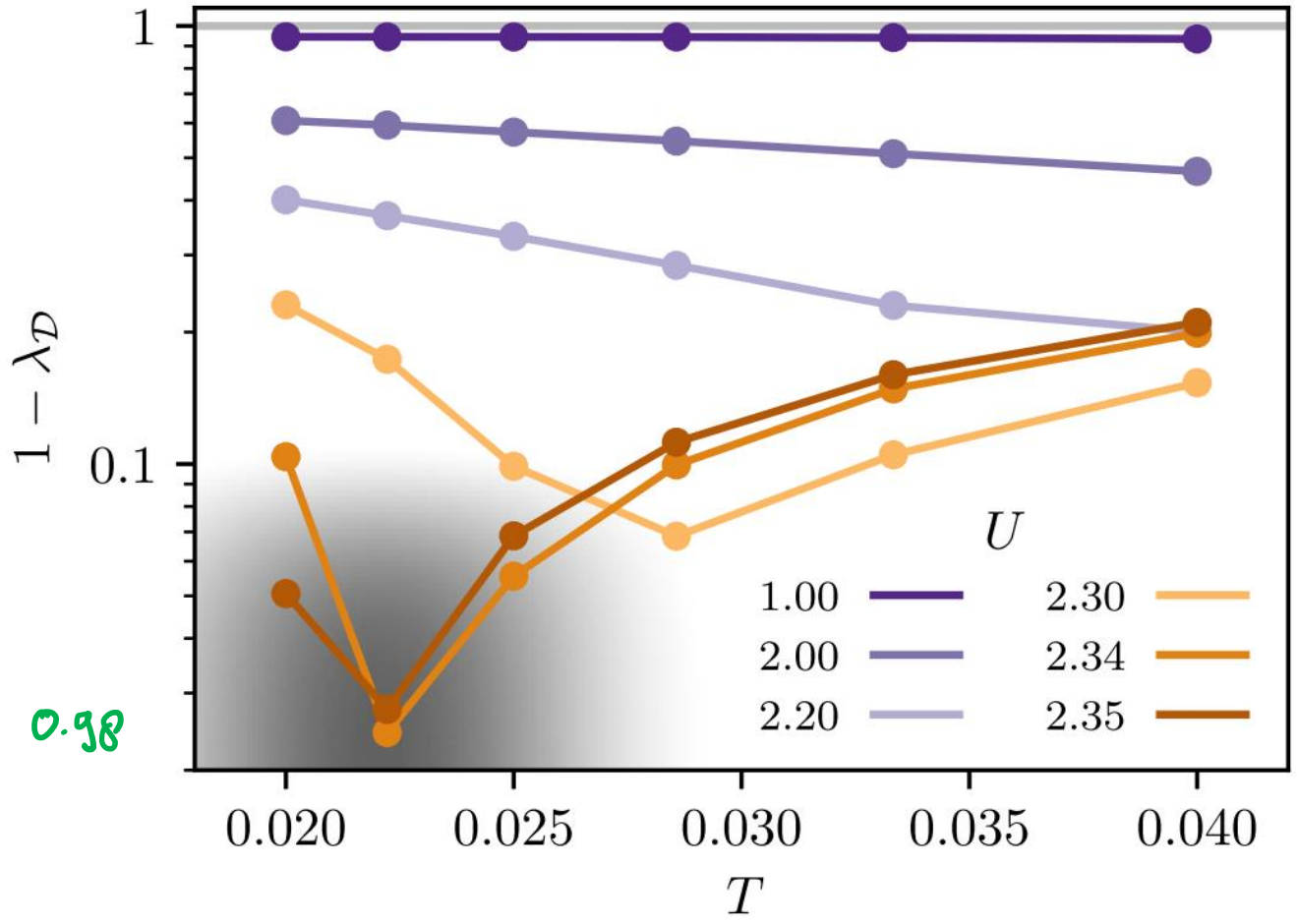
- Compressibility (thermodynamic stability)
- Iterative stability
- Free energy maximum/minimum



- DMFT instabilities are all about non-local feedback

- What happens at the Mott transition?

Leading eigenvalue



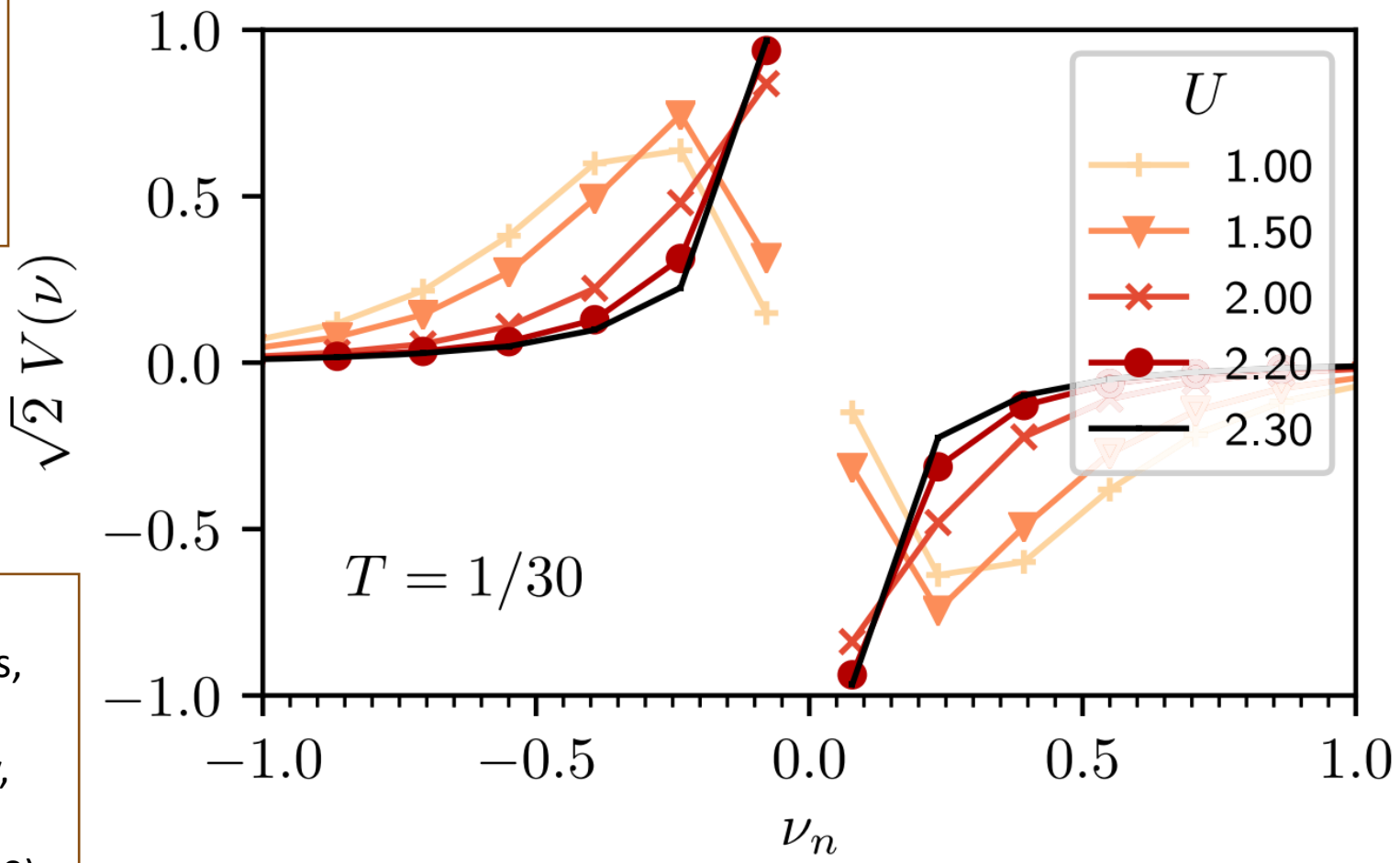
Note:
Single, physical divergence

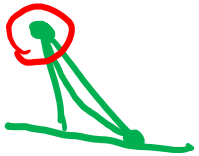
Eigenvectors (normalized)

As the transition is approached, weight of this eigenvector moves to the lowest Matsubara frequency

This is the “order parameter” of the transition

Useful to know for diagrammatic theories, e.g., single frequency approach of Astretsov, Rohringer & Rubtsov, PRB **101**, 075109 (2020)

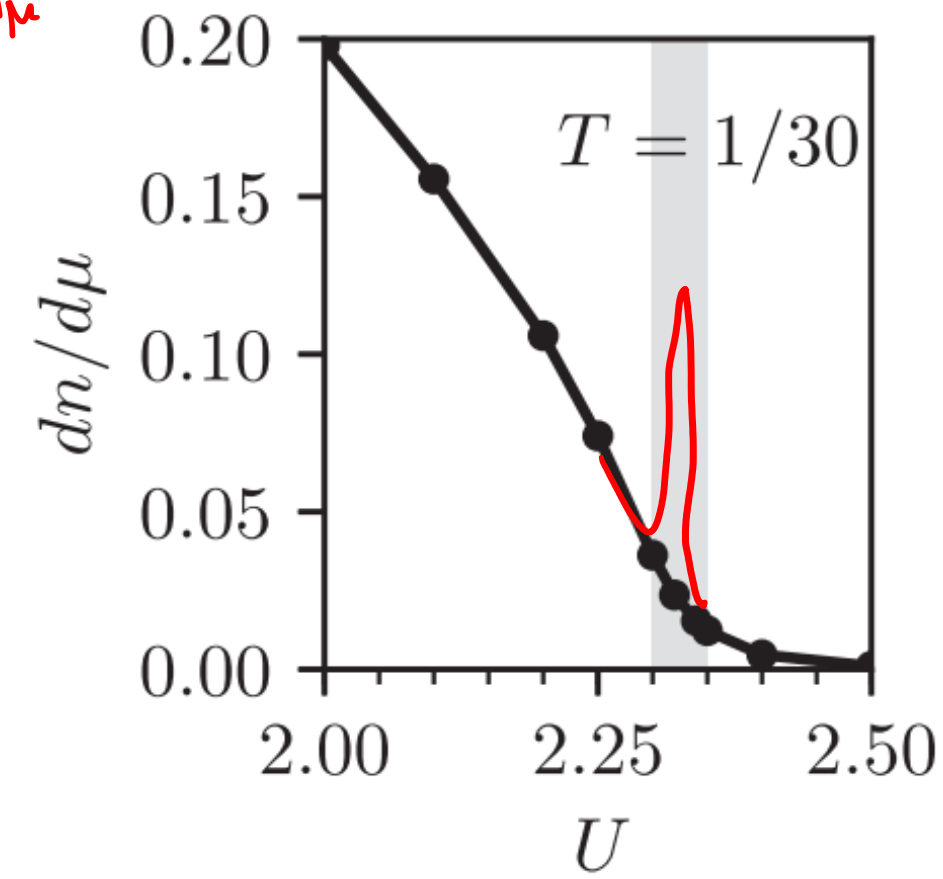




Anti-symmetric in frequency, see D. Springer et al., PRB **101**, 155148 (2020)

Compressibility

Nothing happens?!



Eigenvector anti-symmetric in frequency, see D. Springer et al., PRB **101**, 155148 (2020)

Perspective

$$G^{\sigma}_{\alpha\beta}(w) = \langle c^{\dagger}_{\alpha\sigma} c_{\beta\sigma} \rangle_w$$

$$G^{(2)\,\sigma\sigma'}_{\alpha\beta\gamma\delta}(w,w',\Omega) = \langle c^{\dagger}_{\alpha\sigma} c_{\beta\sigma} c^{\dagger}_{\gamma\sigma'} c_{\delta\sigma'} \rangle (w,w',\Omega)$$

Huge matrix objects. How much of that data is interesting and useful? How much information is contained in these matrices?

huge matrix → metal or insulator

Perspective: Bethe-Salpeter equation

- Eigenvectors of the Bethe-Salpeter equation show the relative importance of Matsubara frequencies for the metal-insulator transition
- In general, they show *relevant* fluctuations (soft modes).
- Information content of the Green's function, where and how is information contained,
  - Compression (e.g., Markus Wallerberger talk).
  - Physics based, not just mathematics based.
  - More efficient calculations possible, important with an eye on DMFT+molecular dynamics, potential energy surfaces, etc., where many similar calculations are done.

universality

$$\Delta_\nu = \sum_{\nu'} V_{\nu'}(\nu)$$

V_0

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