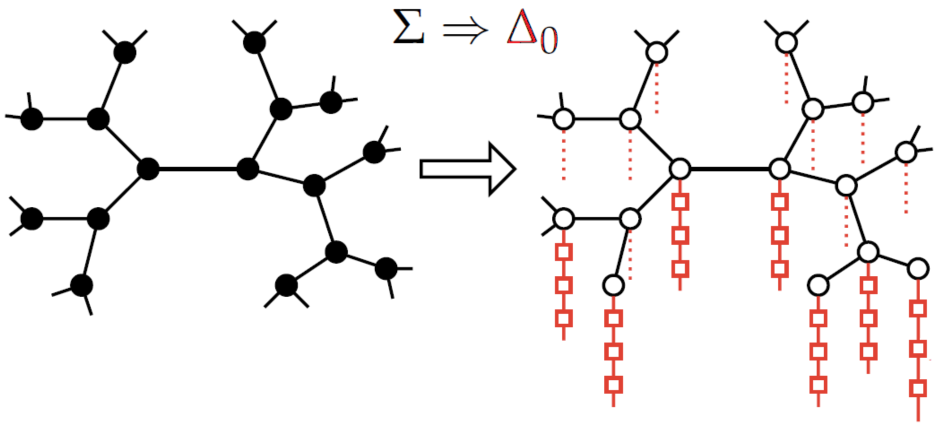
The Mott transition as a topological phase transition



Andrew Mitchell

with Sudeshna Sen and Patrick Wong

University College Dublin

PRB 102, 081110(R) (2020)

IRISH RESEARCH COUNCIL

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Mott topology

Mott transition:

Metal-insulator transition in the Hubbard model and self-energy structure

Topological phase transitions:

Su-Schrieffer-Heeger (SSH) model, boundary Green's functions, and domain walls

Auxiliary field mapping:

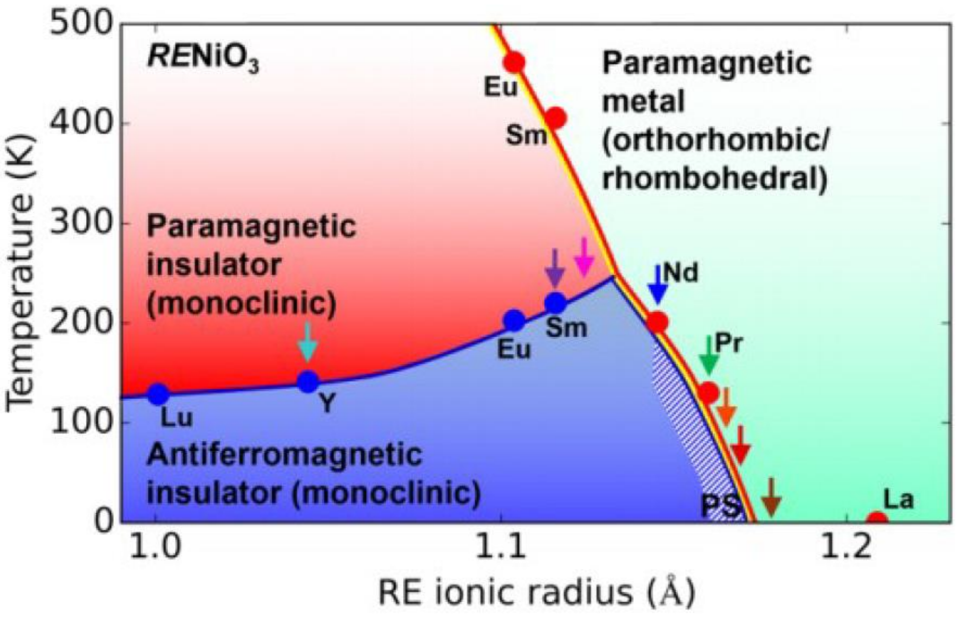
Exact dynamics reproduced in a fully non-interacting system

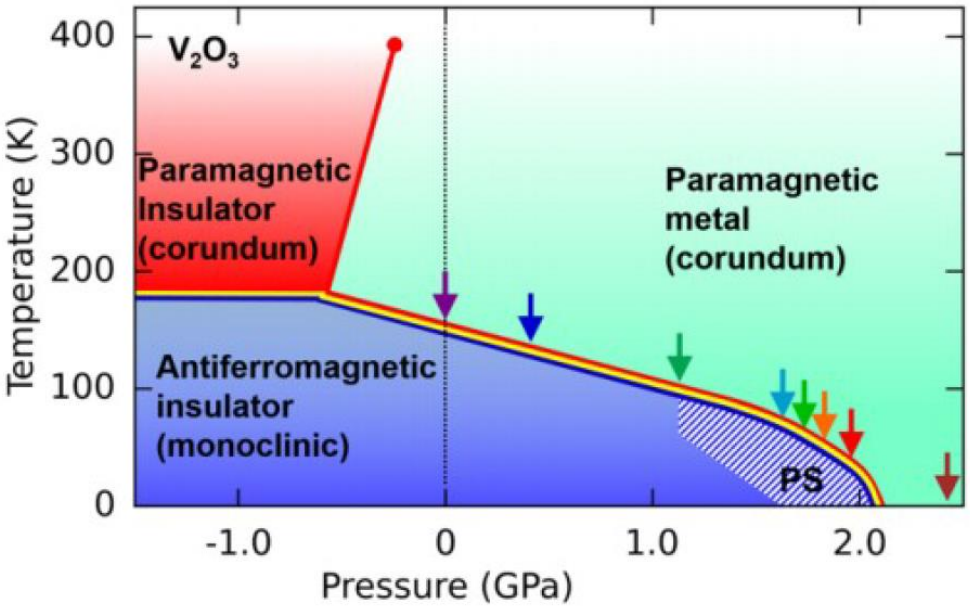
Topological properties of the auxiliary system:

Exact dynamics reproduced in a fully non-interacting system

Mott transition

Metal-insulator transition driven by electronic interactions



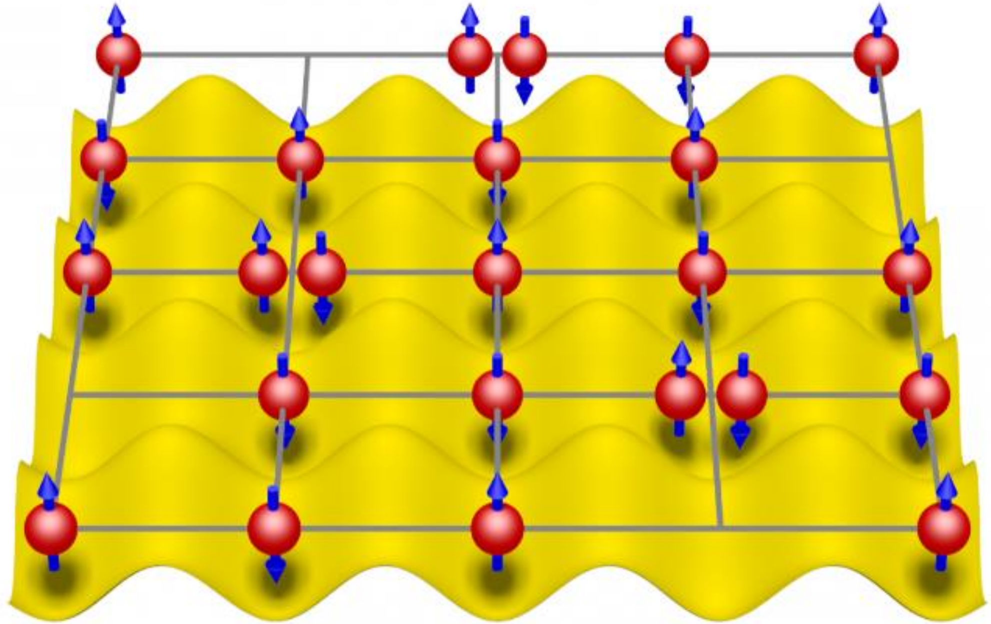


See e.g. RMP 70, 1039 (1998); Nature Comms 7, 12519 (2016)

Hubbard Model

Local Coulomb repulsion competes with tunneling

$$H = \sum_{i,j,\sigma} \left[t_{ij}\, c^{\dagger}_{i,\sigma} c_{j,\sigma} \right] + U \sum_{j} c^{\dagger}_{j,\uparrow} c_{j,\uparrow}\, c^{\dagger}_{j,\downarrow} c_{j,\downarrow}$$



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Hubbard Model

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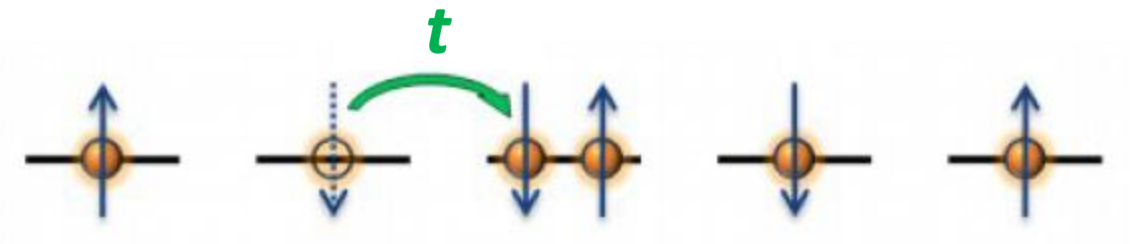
t>>U : metallic

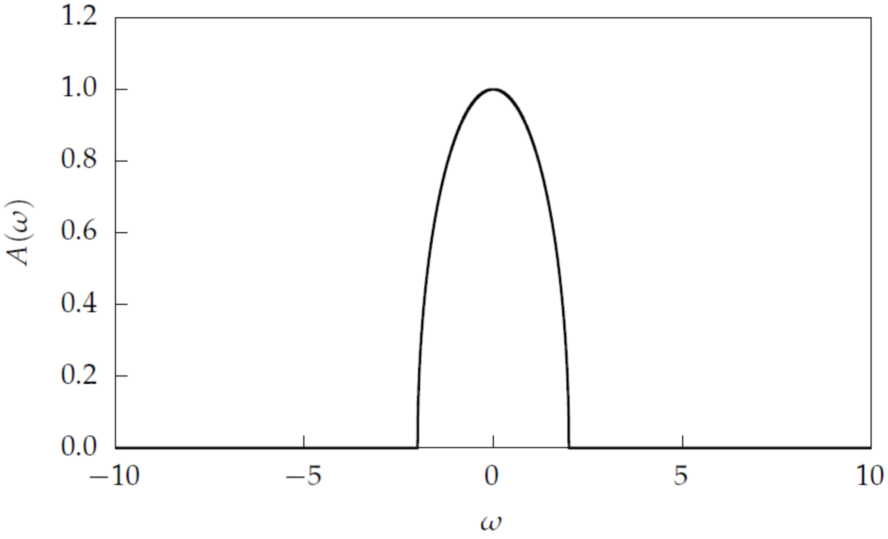


t<<U : insulating

Hubbard Model: metallic phase

t>>U : Treat interaction as a perturbation to tight-binding model

$$H = \sum_{i,j,\sigma} \left[t_{ij}\, c^{\dagger}_{i,\sigma} c_{j,\sigma} \right]$$



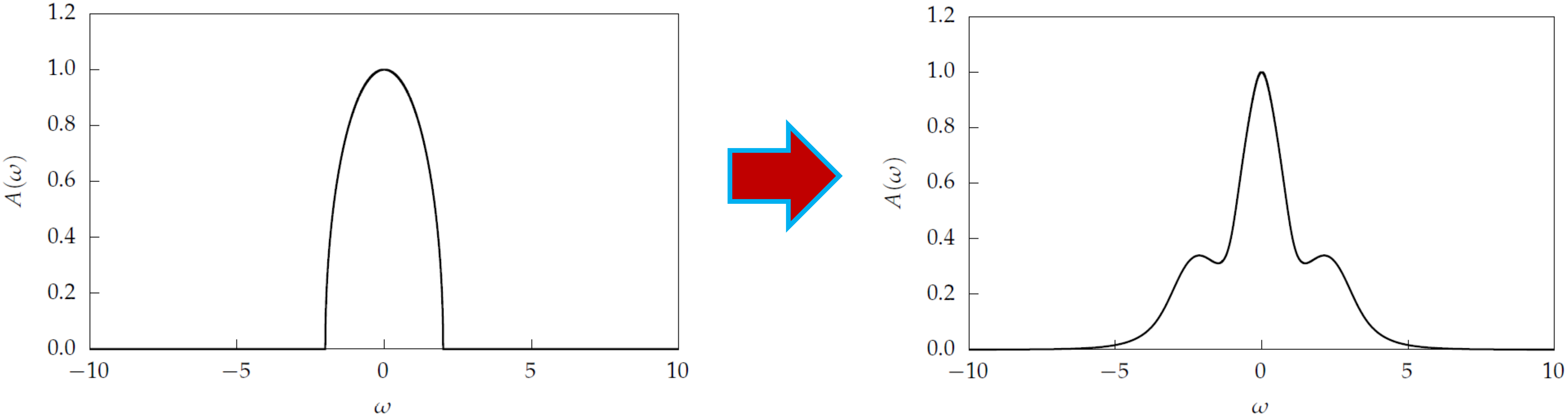
$$G^0_{loc}(\omega) = \frac{1}{\omega^+ + \mu - \Delta(\omega)}$$

$$A^0_{loc}(\omega) = -\frac{1}{\pi} \mathrm{Im}\, G^0_{loc}(\omega)$$

Hubbard Model: metallic phase

t>>U : Treat interaction as a perturbation to tight-binding model

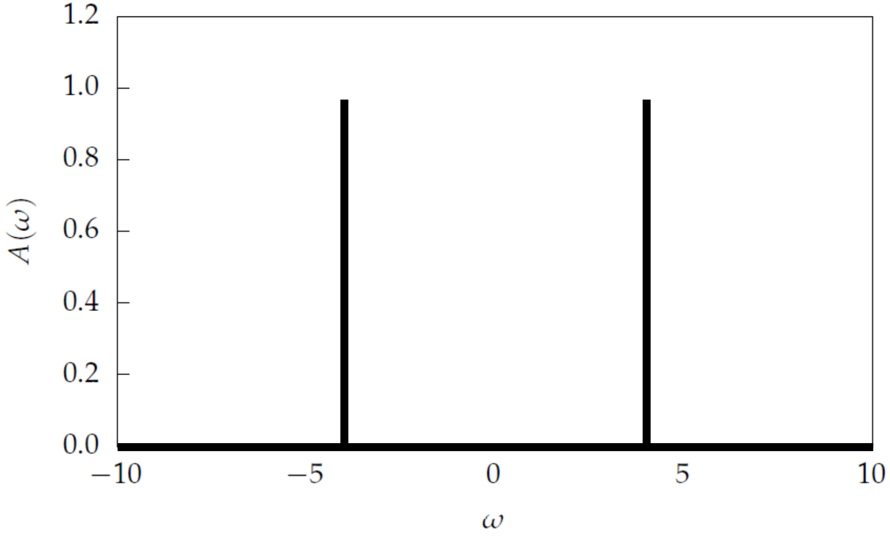
$$H = \sum_{i,j,\sigma} \left[t_{ij} \; c^{\dagger}_{i,\sigma} c_{j,\sigma} \right] + H'$$



Hubbard Model: insulating phase

U>>t : Treat hopping as a perturbation to "atomic limit"

$$H = U\sum_j c^\dagger_{j,\uparrow}c_{j,\uparrow}\, c^\dagger_{j,\downarrow}c_{j,\downarrow}$$



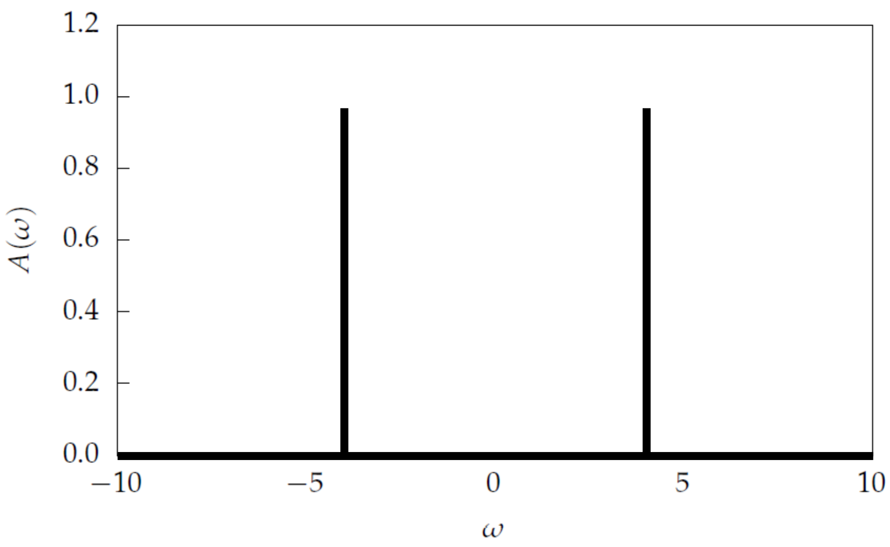
$$G_{loc}(\omega) = \frac{1}{\omega^+ + \mu - \Sigma(\omega)}$$

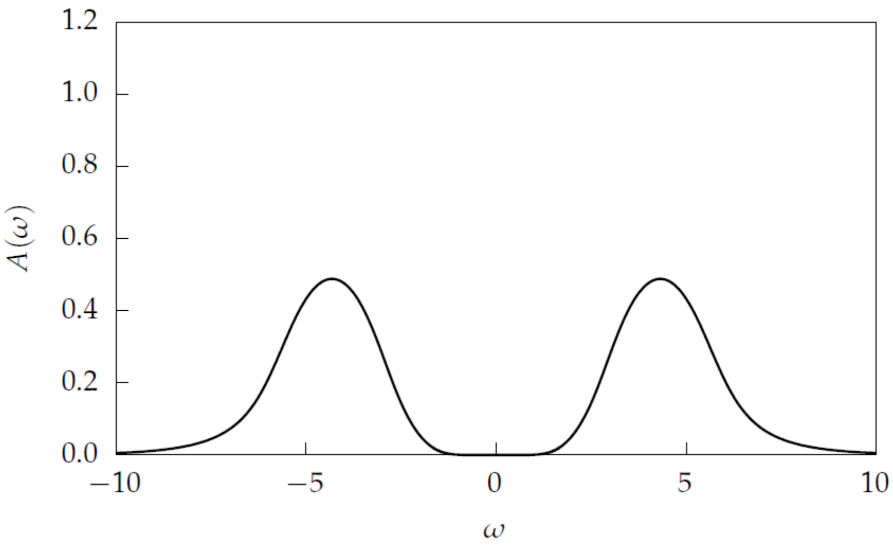
$$\Sigma(\omega) = \frac{U}{2} + \frac{(U/2)^2}{\omega^+ + \mu - U/2}$$

Hubbard Model: insulating phase

U>>t : Treat hopping as a perturbation to "atomic limit"

$$H = U \sum_j c^\dagger_{j,\uparrow} c_{j,\uparrow} c^\dagger_{j,\downarrow} c_{j,\downarrow} + H'$$





Mott transition

U ~ t : Non-perturbative

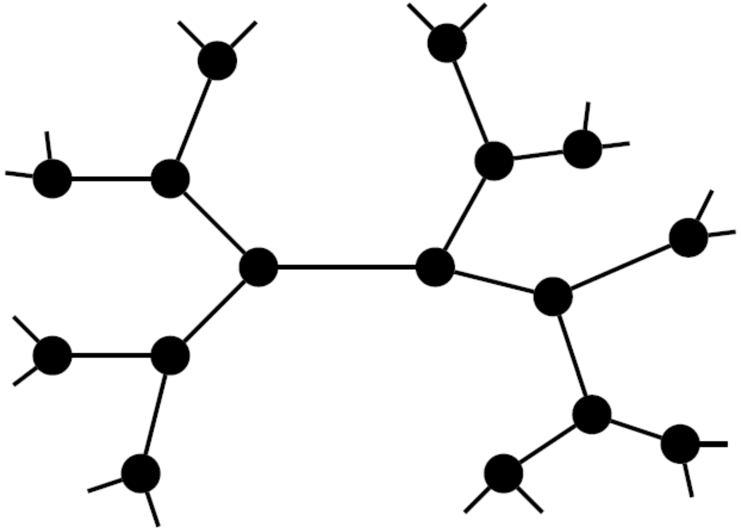
$$H = \sum_{i,j,\sigma} \left[t_{ij}\, c^\dagger_{i,\sigma} c_{j,\sigma} \right] + U \sum_{j} c^\dagger_{j,\uparrow} c_{j,\uparrow}\, c^\dagger_{j,\downarrow} c_{j,\downarrow}$$

➡ **metal-insulator transition!**

Dynamical Mean Field Theory (DMFT)

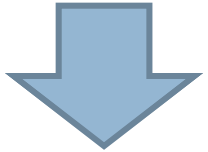
One-band Hubbard model on the infinite-dimensional Bethe lattice

$$H = \sum_{i,j,\sigma} \left[t_{ij}\ c^{\dagger}_{i,\sigma} c_{j,\sigma} \right] + U \sum_{j} c^{\dagger}_{j,\uparrow} c_{j,\uparrow}\ c^{\dagger}_{j,\downarrow} c_{j,\downarrow}$$



PRL 62, 324 (1989)

Local self-energy



DMFT

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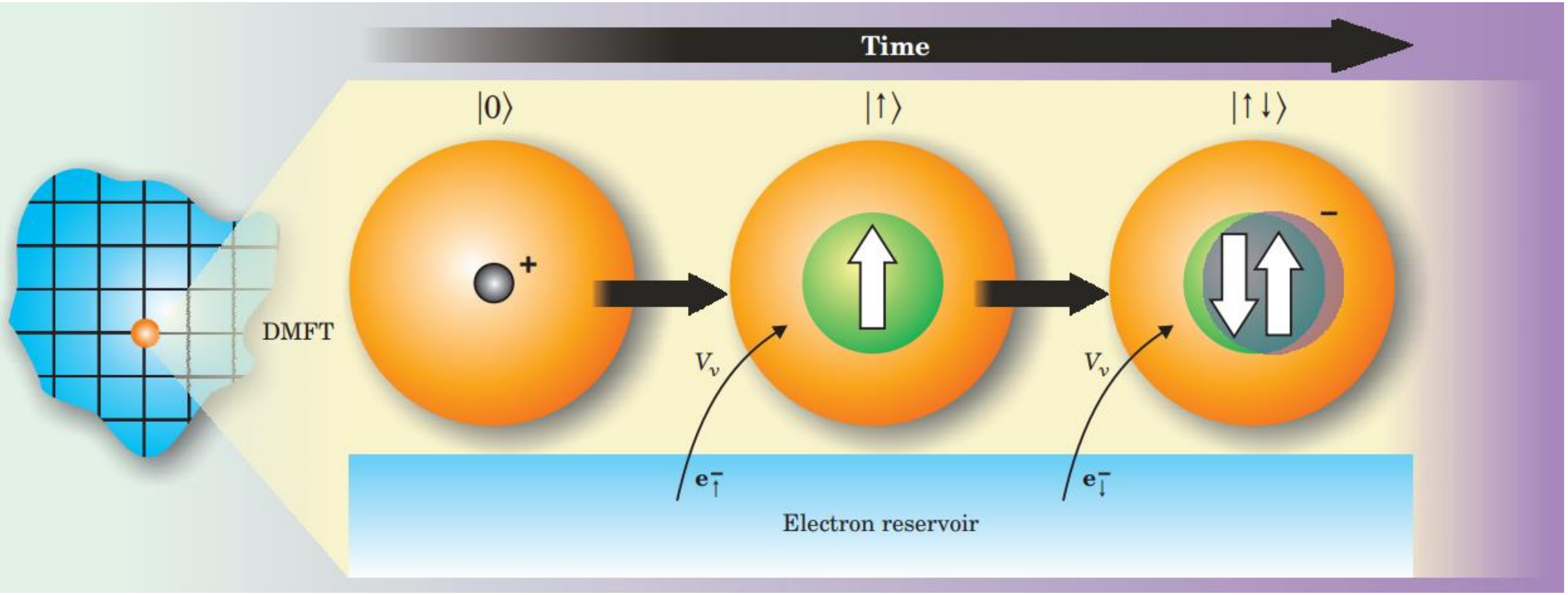
Dynamical Mean Field Theory (DMFT)

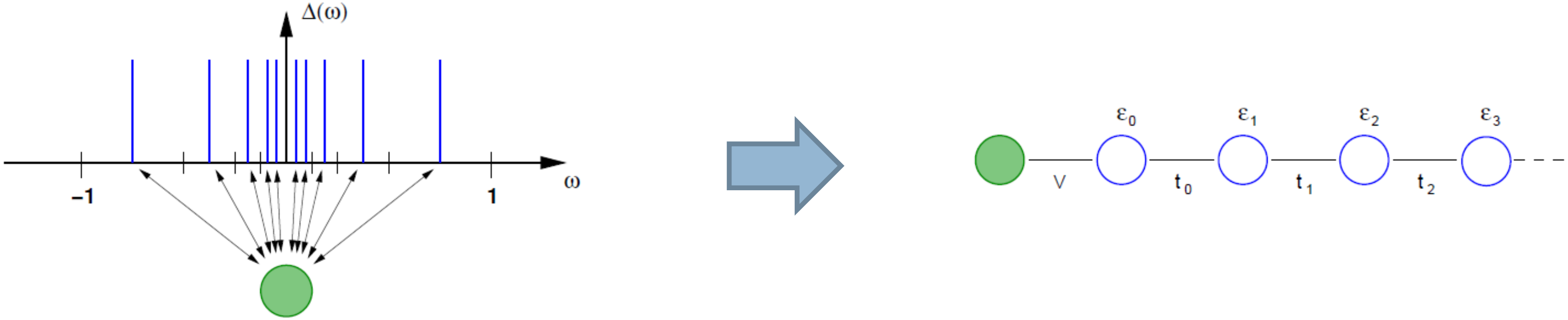
Hubbard model mapped to a single-impurity Anderson model



See e.g. RMP 68,13, (1996); Physics Today 57, 53 (2004)

Numerical Renormalization Group (NRG)

Impurity problem solved numerically-exactly using NRG



See e.g. RMP 55, 583 (1983); RMP 80, 395 (2008); PRL 83, 136 (1999)

DMFT-NRG for the Hubbard Model

Lattice problem:

$$G_{latt}(\omega) = [\omega^+ - \epsilon - \Sigma_{latt}(\omega) - t^2 G_{latt}(\omega)]^{-1}$$

Impurity problem:

$$G_{imp}(\omega) = \left[\omega^+ - \epsilon - \Sigma_{imp}(\omega) - \Delta_{imp}(\omega)\right]^{-1}$$

Self-consistency:

$$G_{latt}(\omega) = G_{imp}(\omega)$$

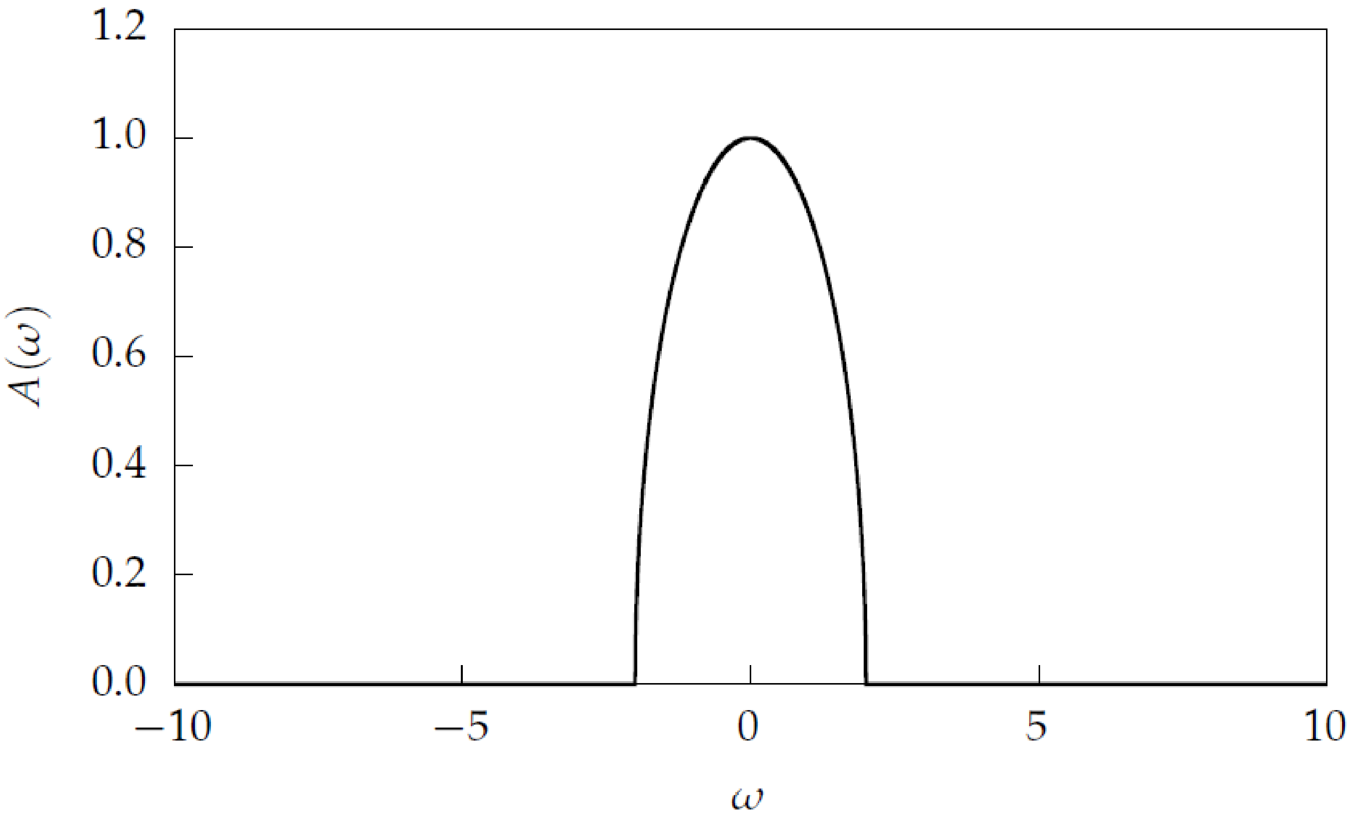
$$\Sigma_{latt}(\omega) = \Sigma_{imp}(\omega)$$

NRG provides accurate $\Sigma_{imp}(\omega)$ for a given $\Delta_{imp}(\omega)$

$\Rightarrow$ zero temperature, high resolution, real frequency

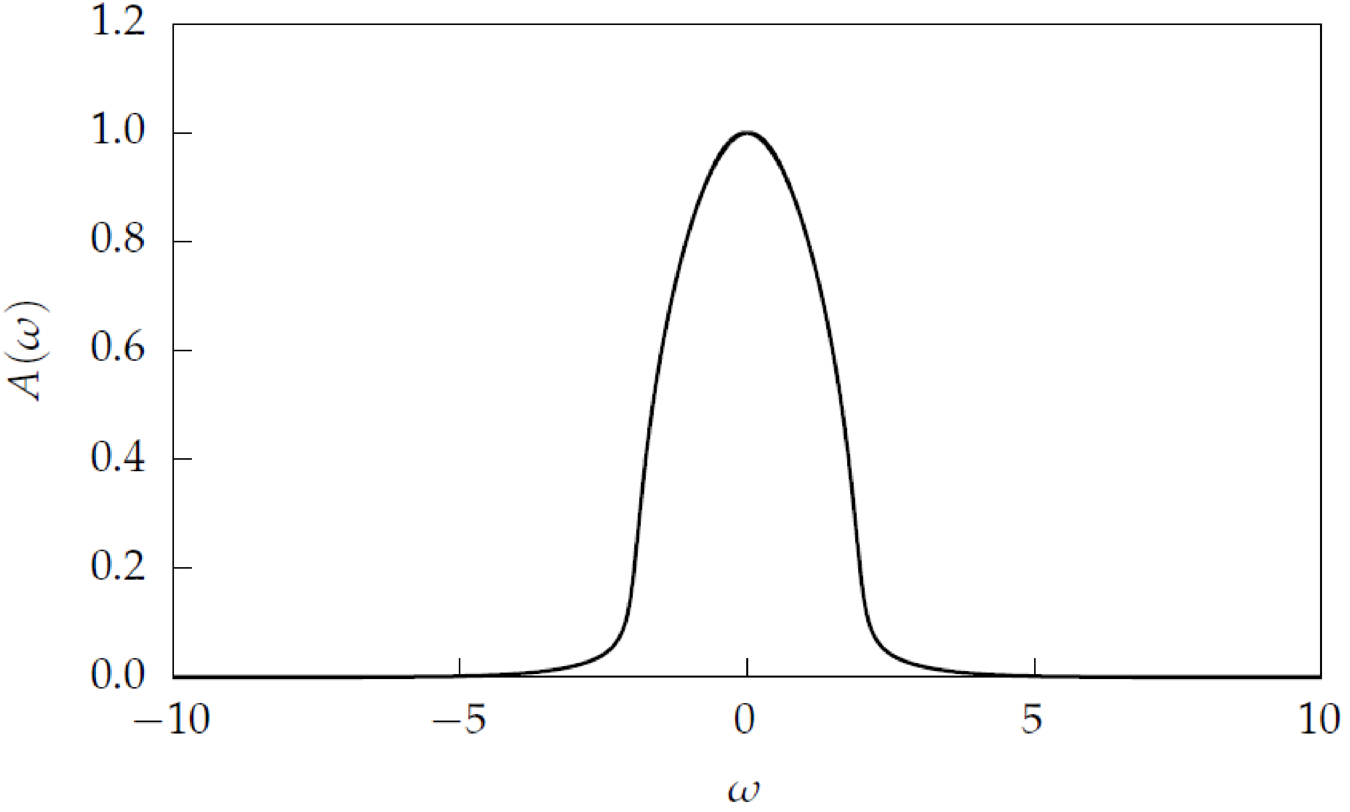
DMFT-NRG for the Hubbard Model

$U/t = 0.0$

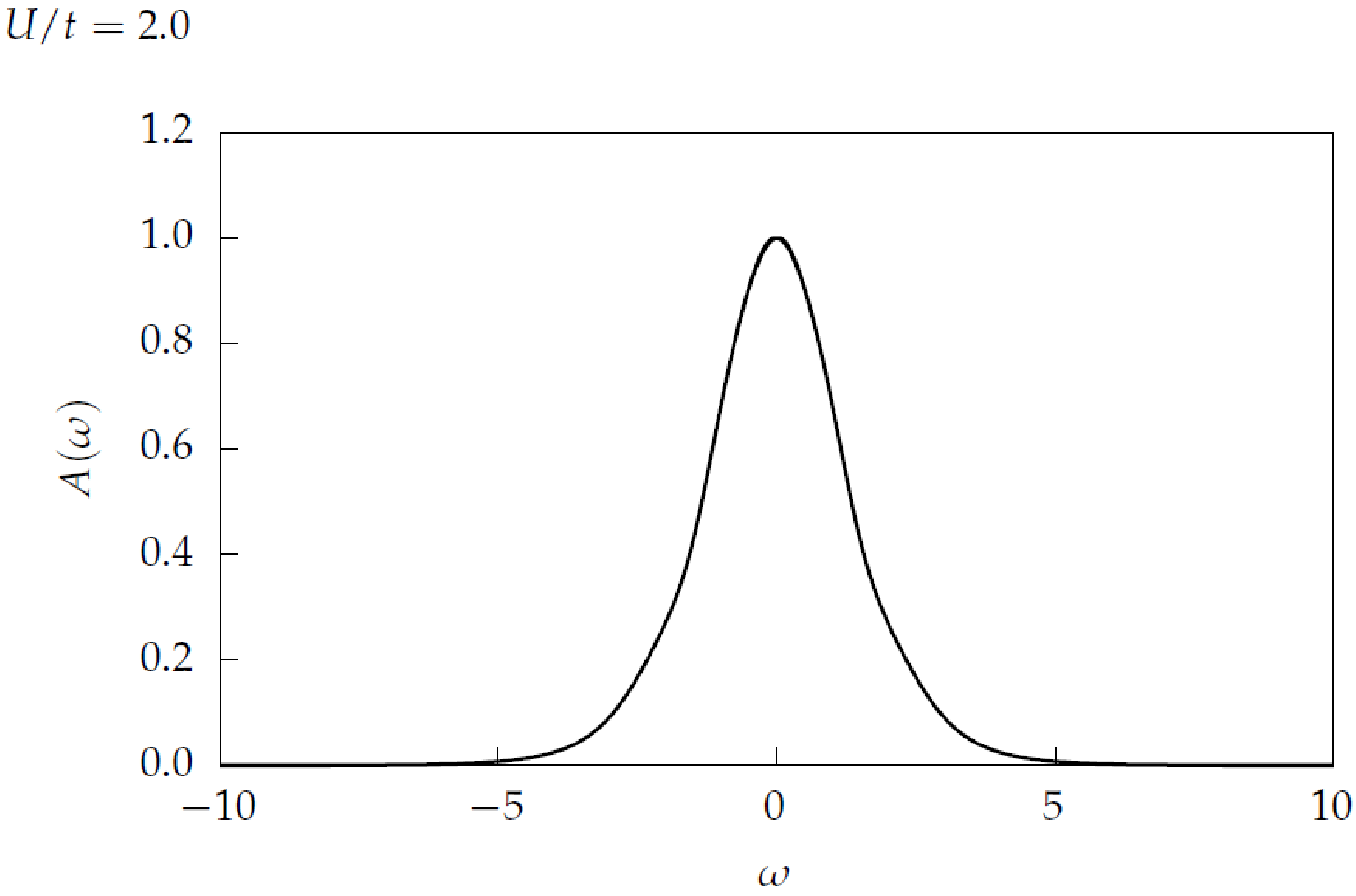


DMFT-NRG for the Hubbard Model

$U/t = 1.0$



DMFT-NRG for the Hubbard Model



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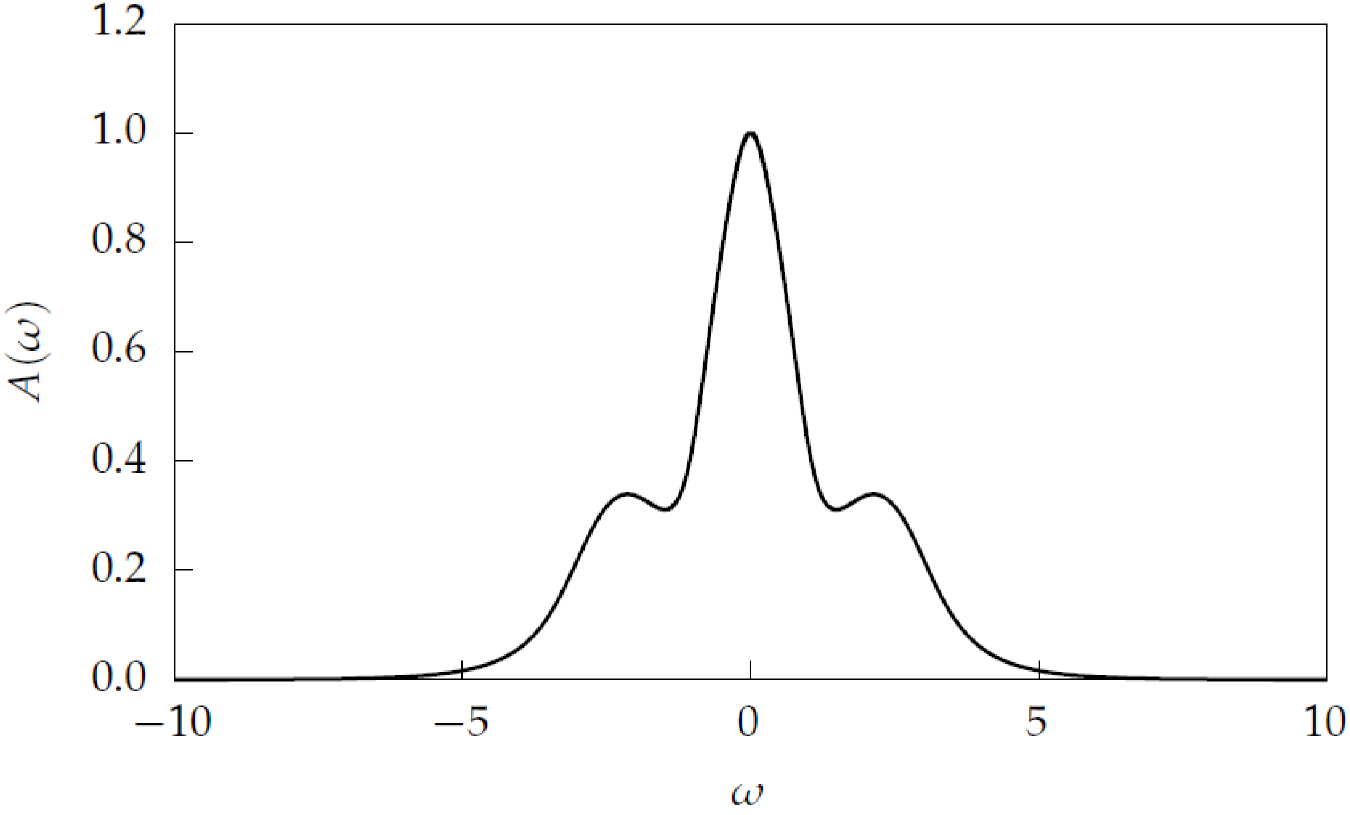
DMFT-NRG for the Hubbard Model

$U/t = 3.0$



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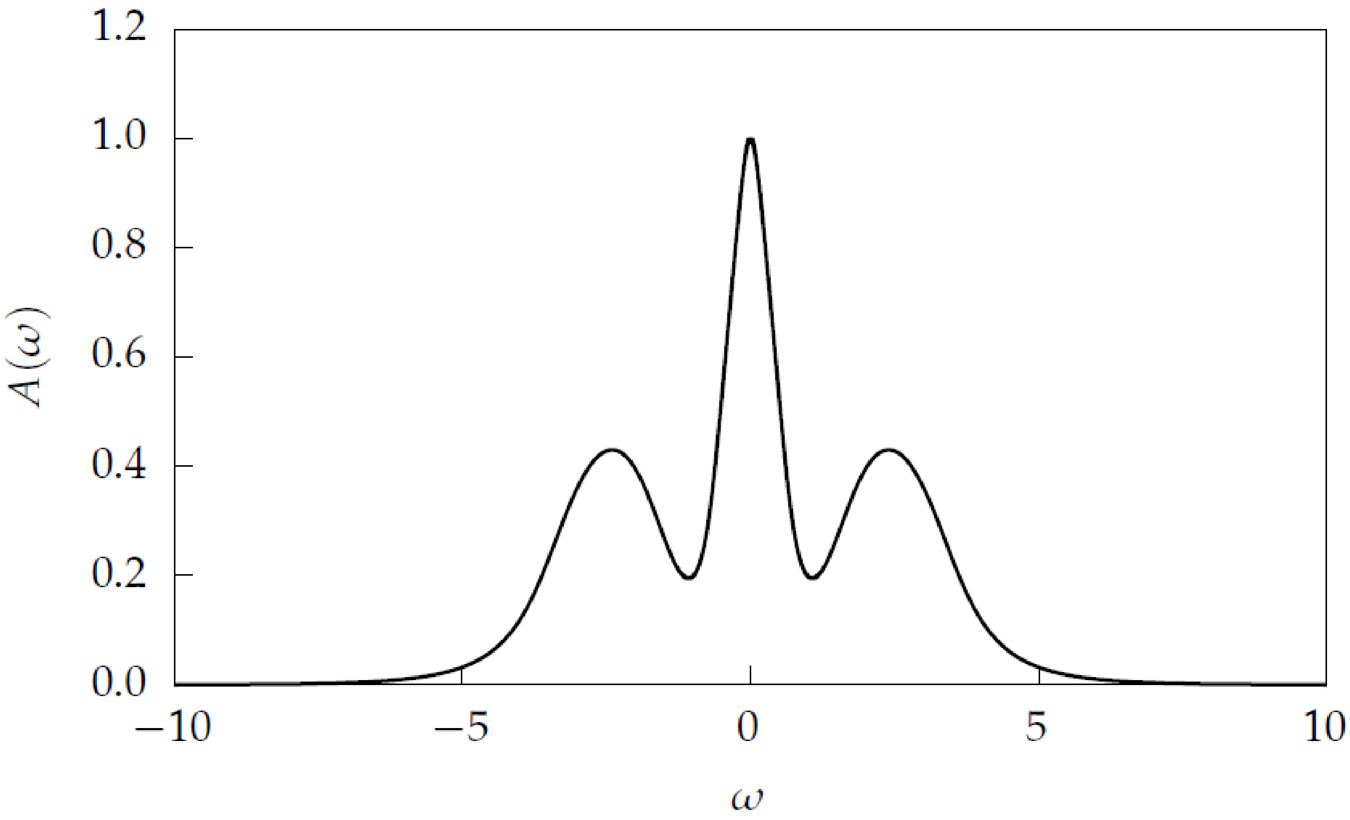
DMFT-NRG for the Hubbard Model

$U/t = 4.0$



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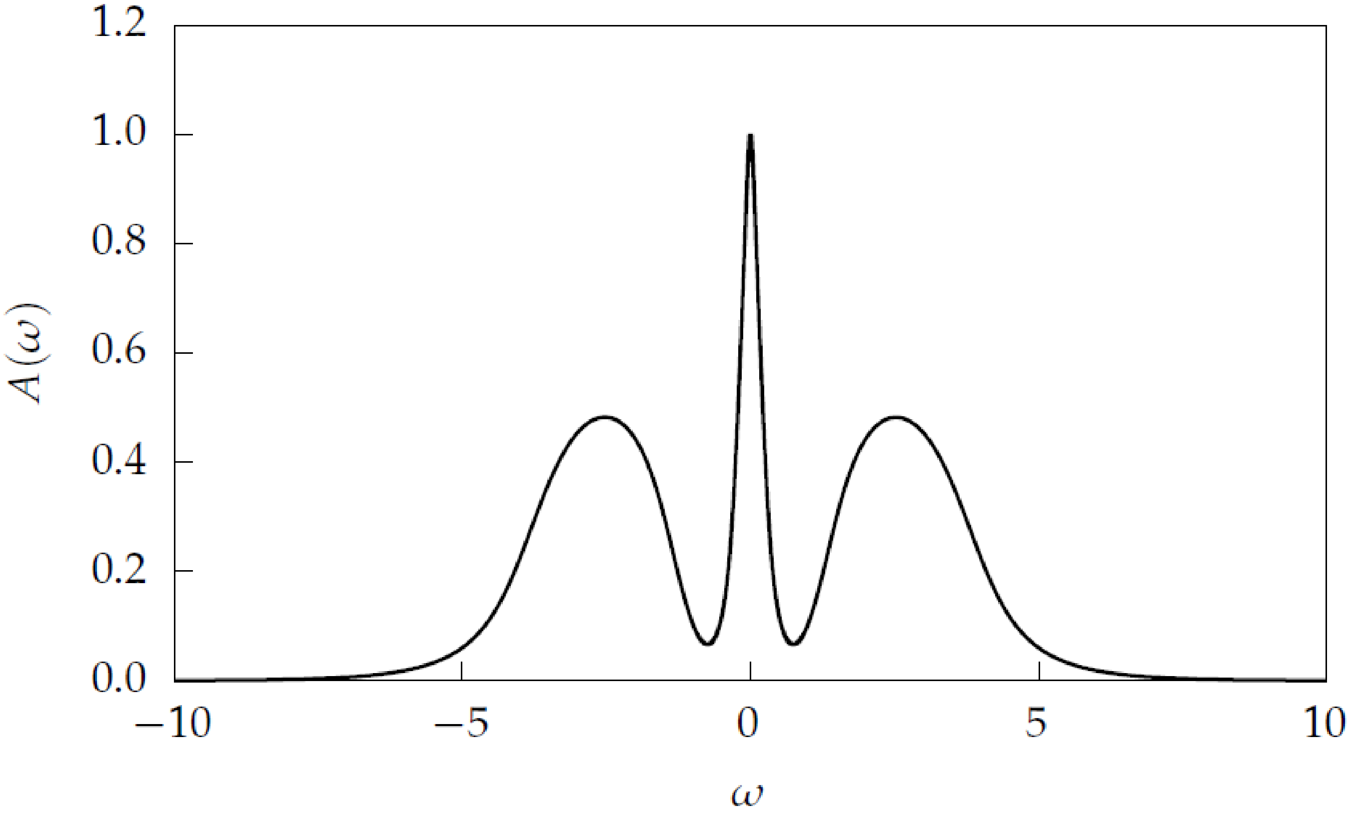
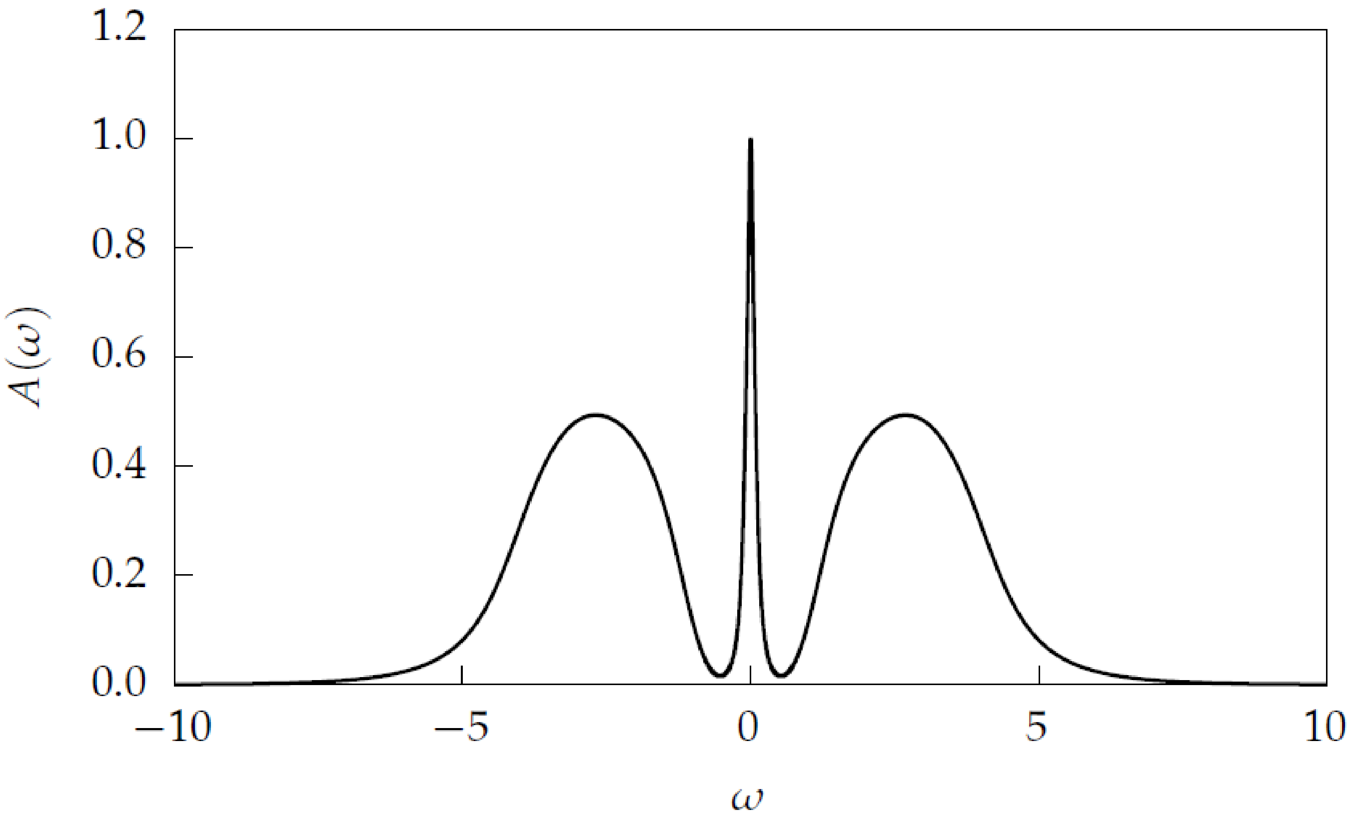
DMFT-NRG for the Hubbard Model

$U/t = 5.0$



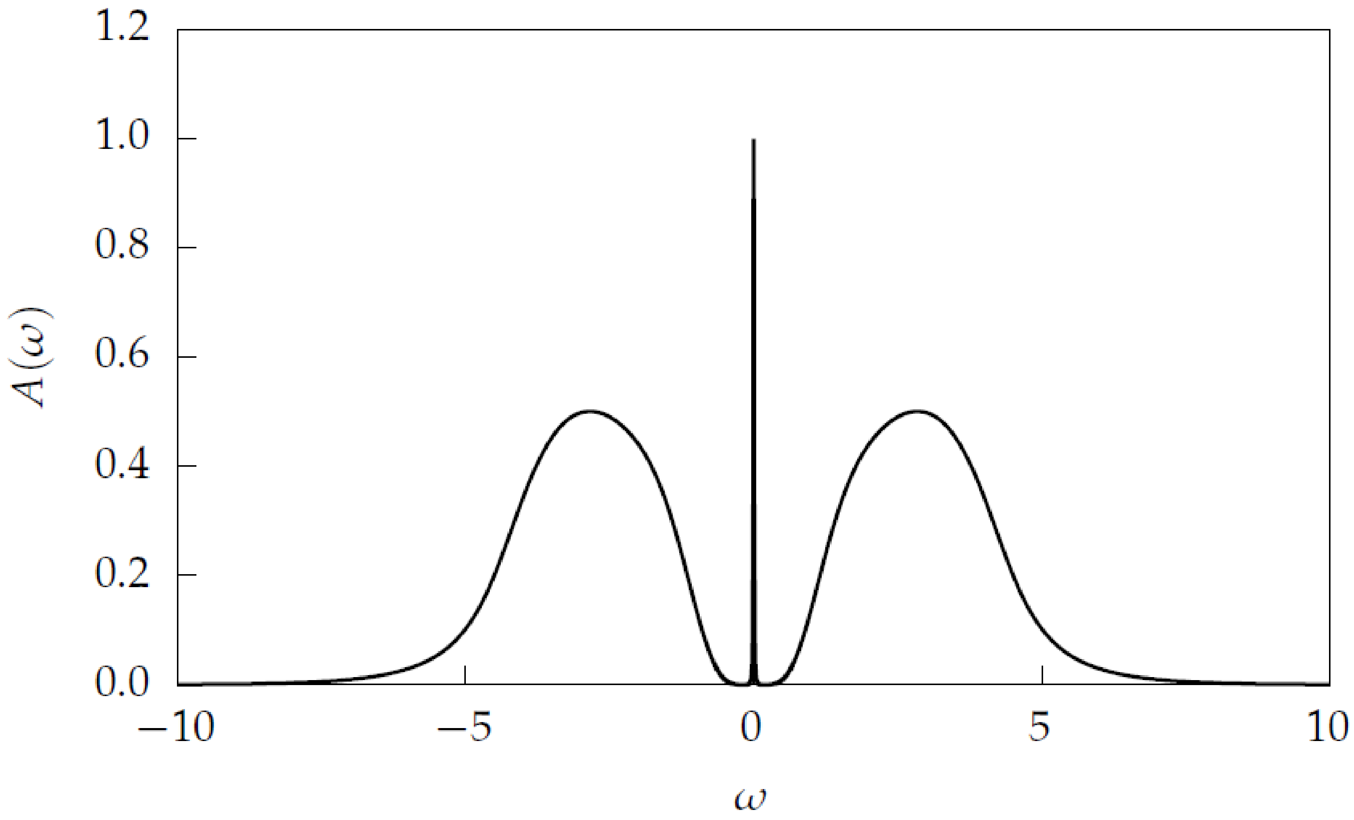
DMFT-NRG for the Hubbard Model

$U/t = 5.5$



DMFT-NRG for the Hubbard Model

$U/t = 5.86$



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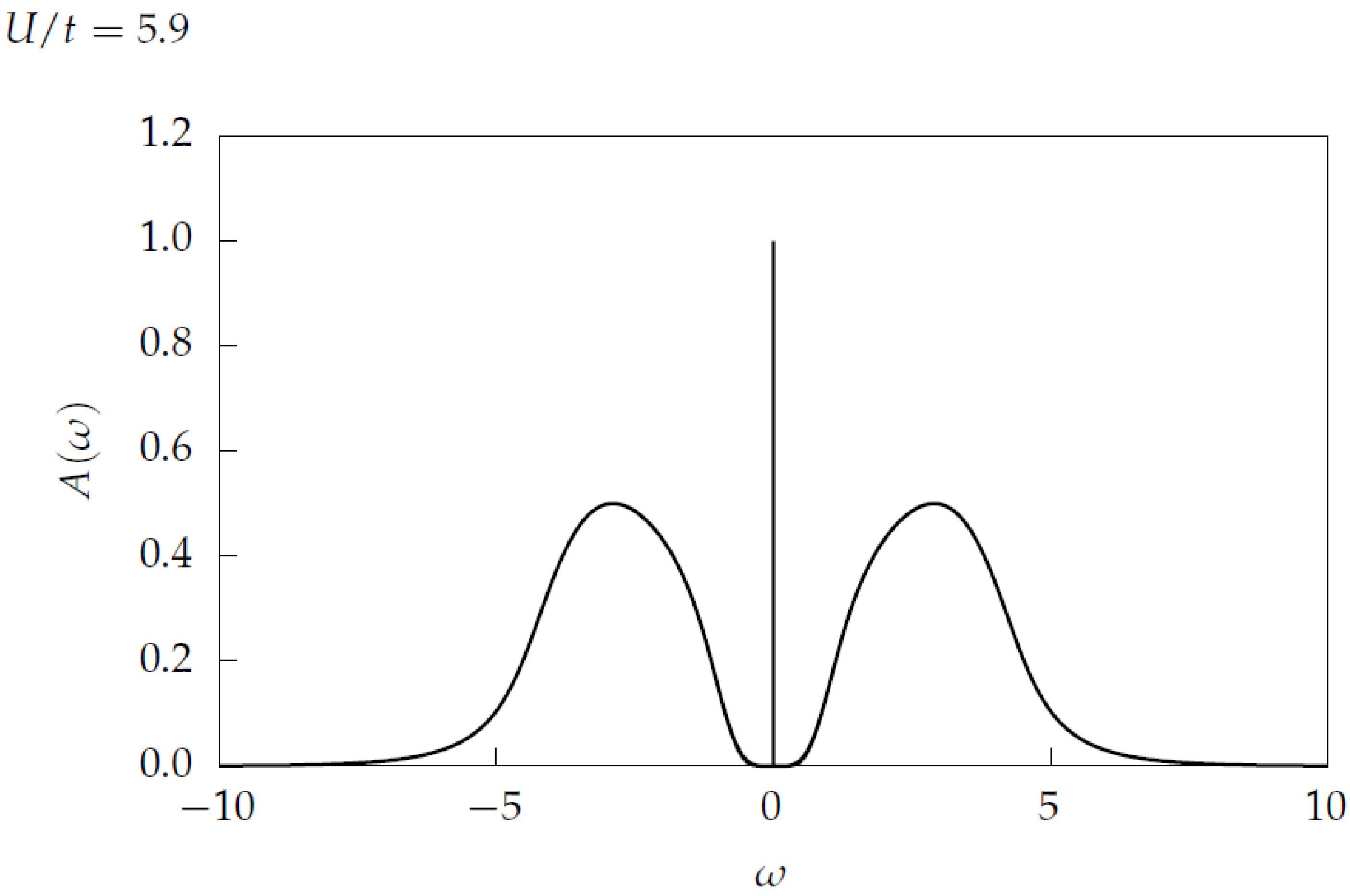
DMFT-NRG for the Hubbard Model



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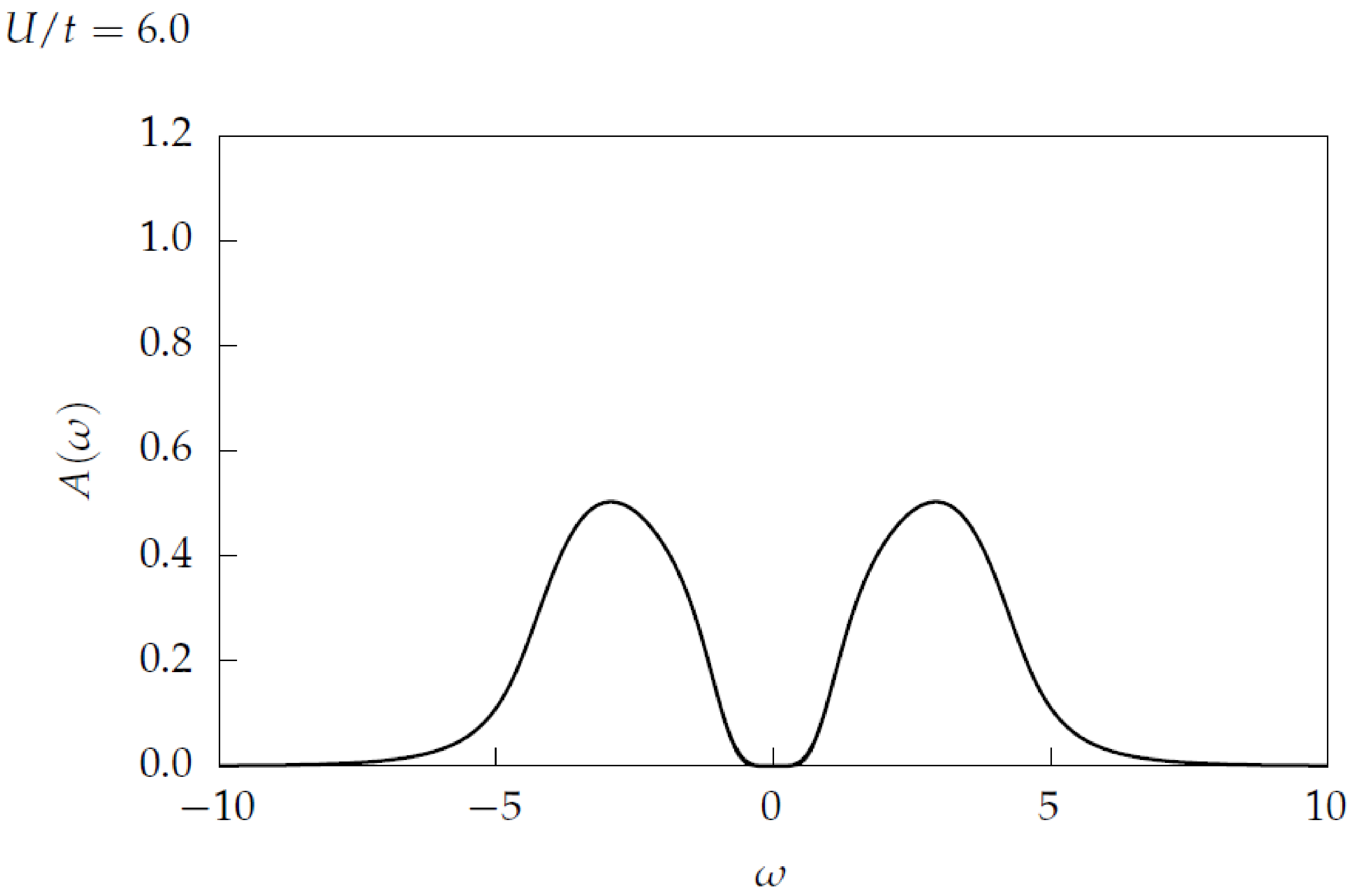
DMFT-NRG for the Hubbard Model



Transition occurs without gap closing

No symmetry breaking

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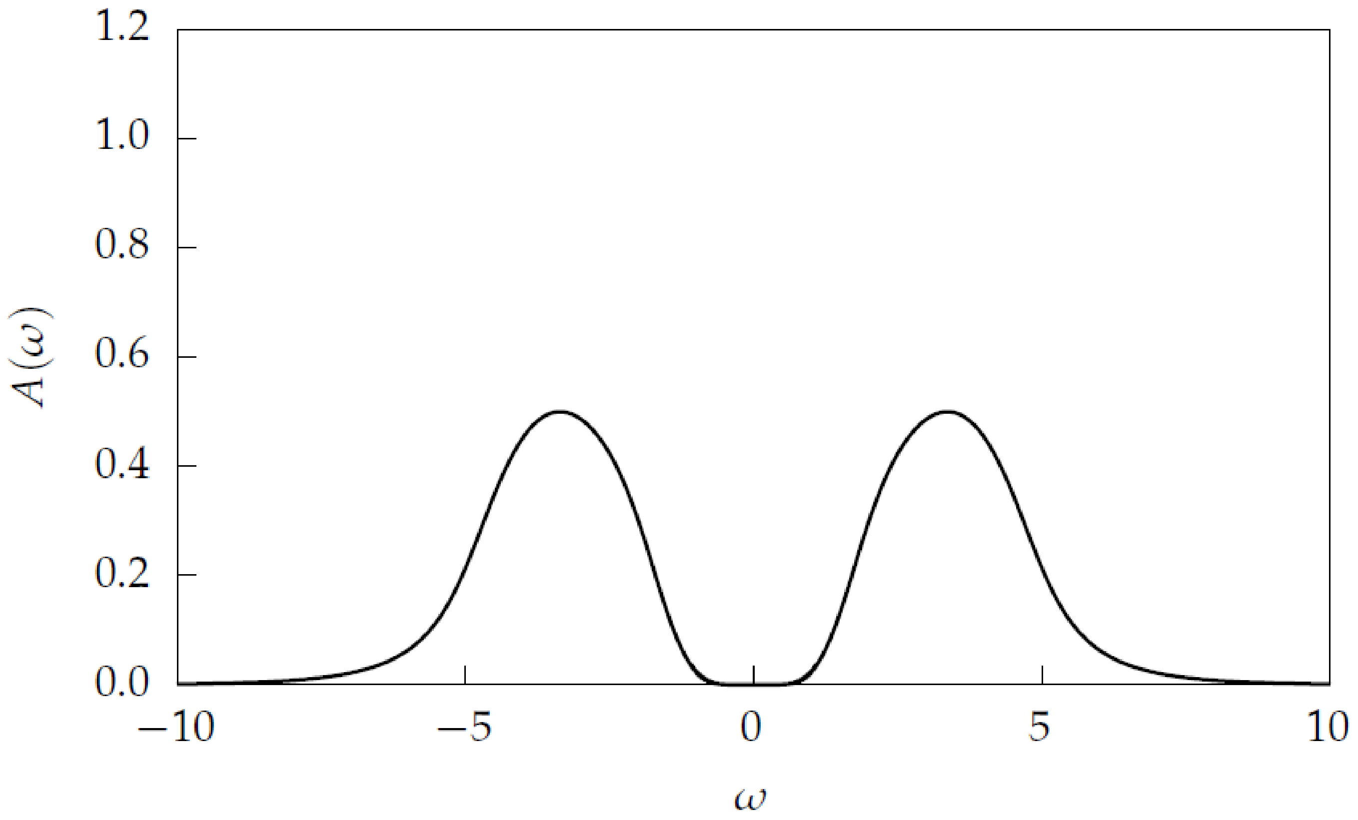
DMFT-NRG for the Hubbard Model

$U/t = 7.0$



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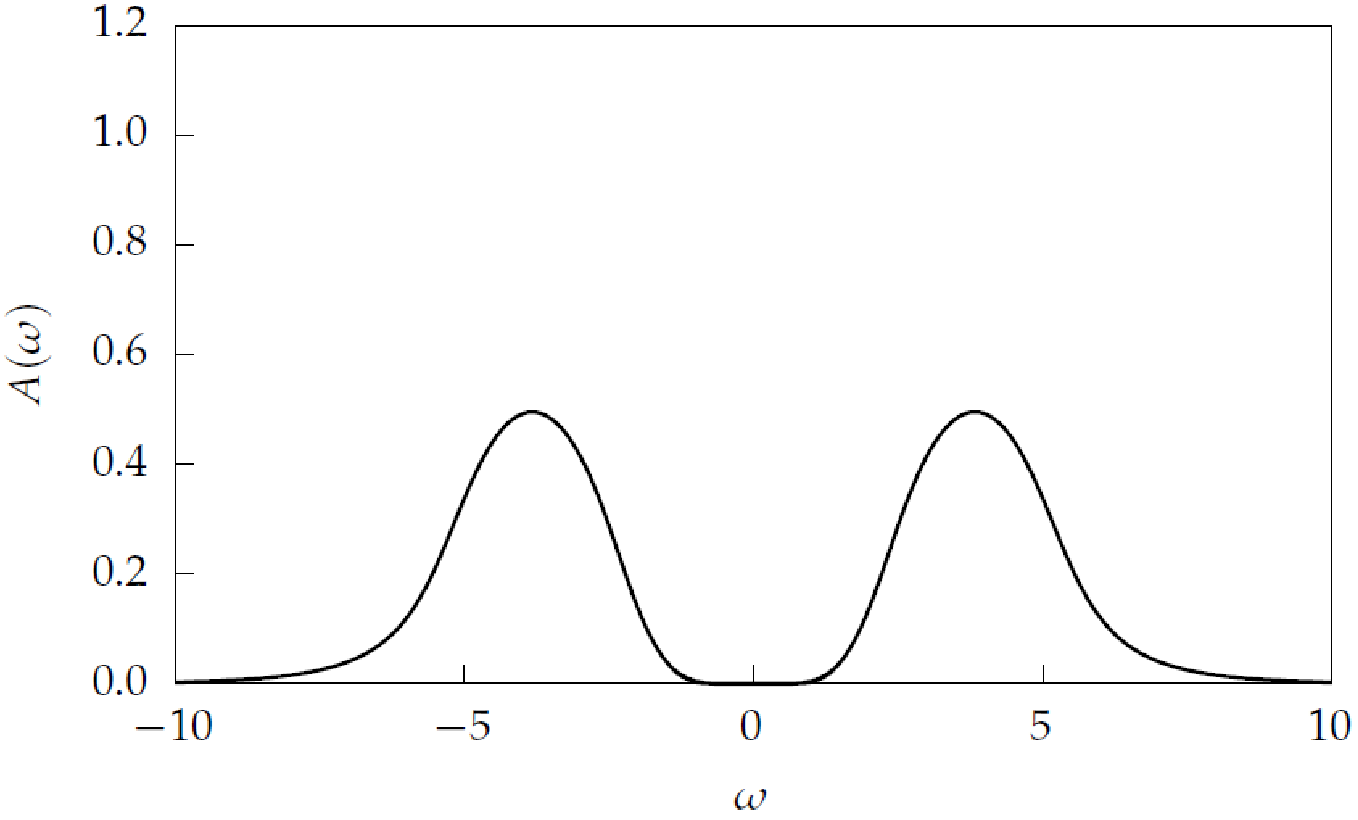
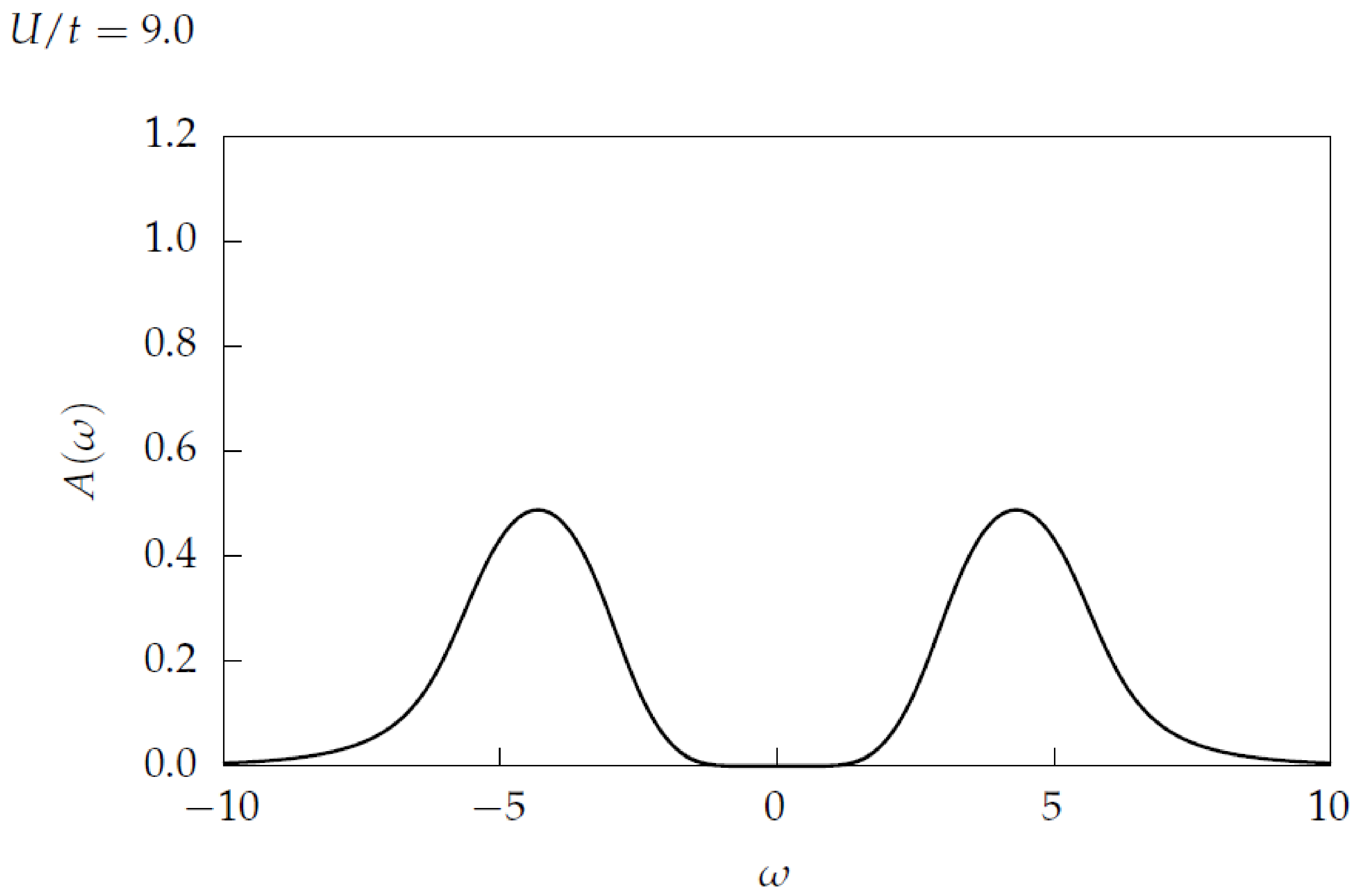
DMFT-NRG for the Hubbard Model

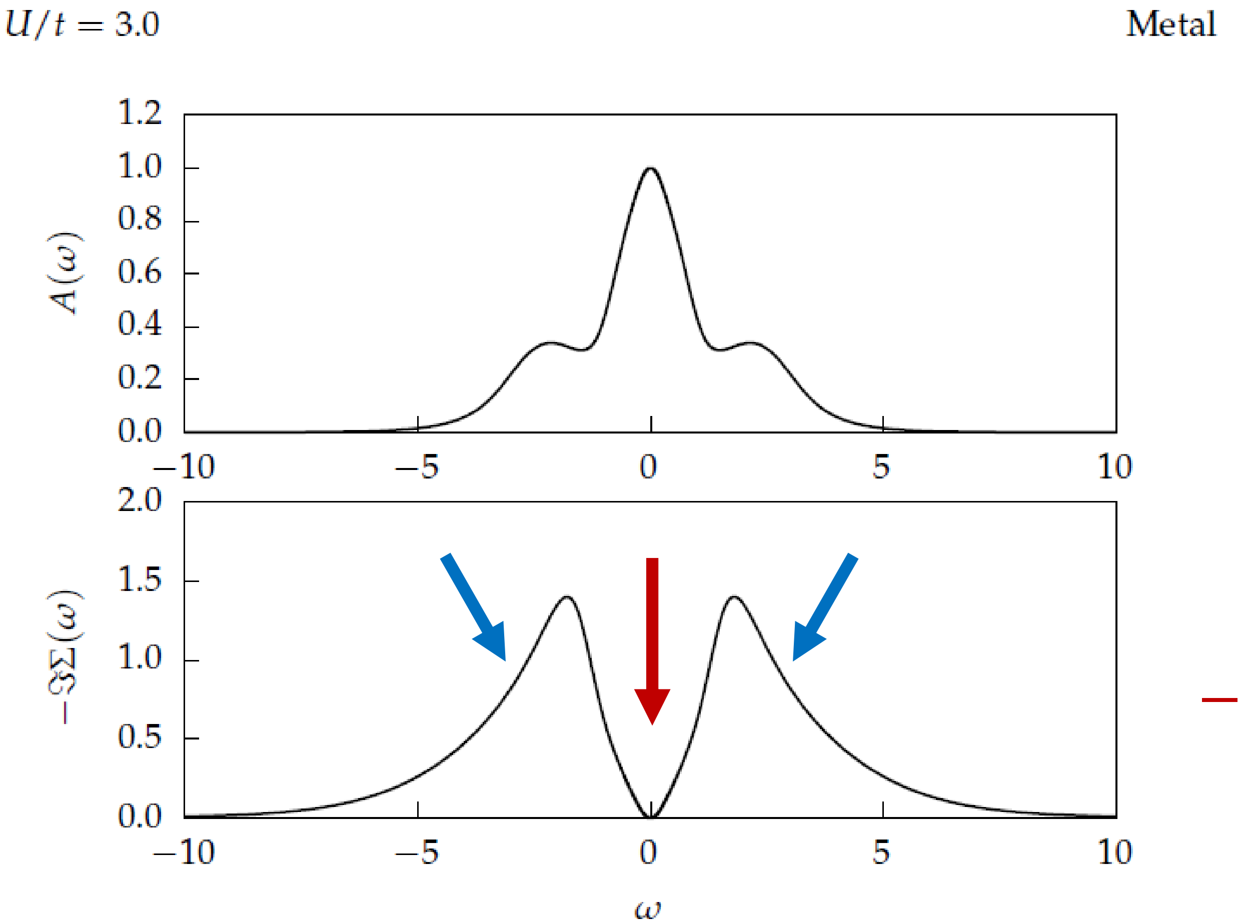
$U/t = 8.0$



DMFT-NRG for the Hubbard Model



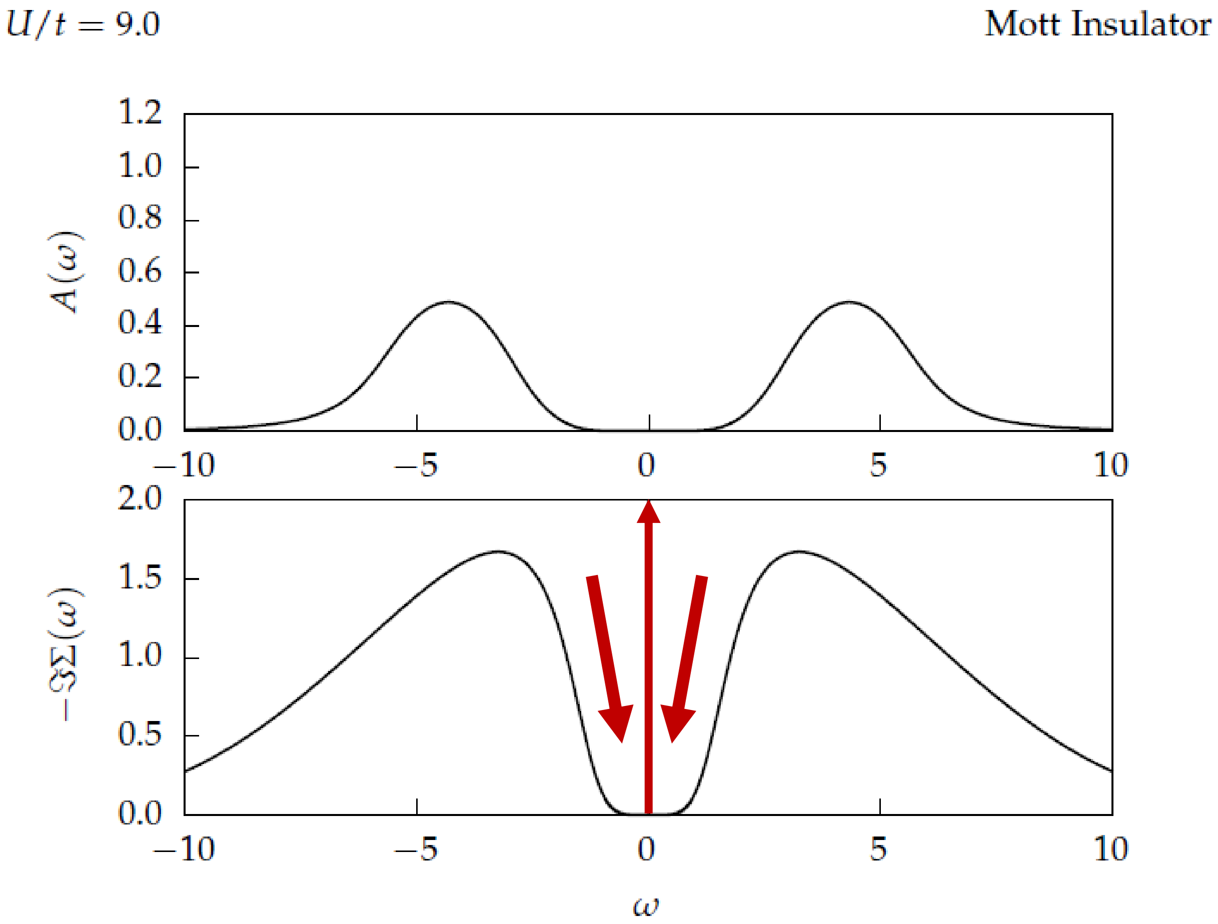
Structure of self-energy



High energies:
Hubbard bands

Low energies:
$-\mathrm{Im}\,\Sigma(\omega) \sim \omega^2$

Structure of self-energy



High energies:

Hubbard bands

Low energies:

Hard gap
+
Mott pole

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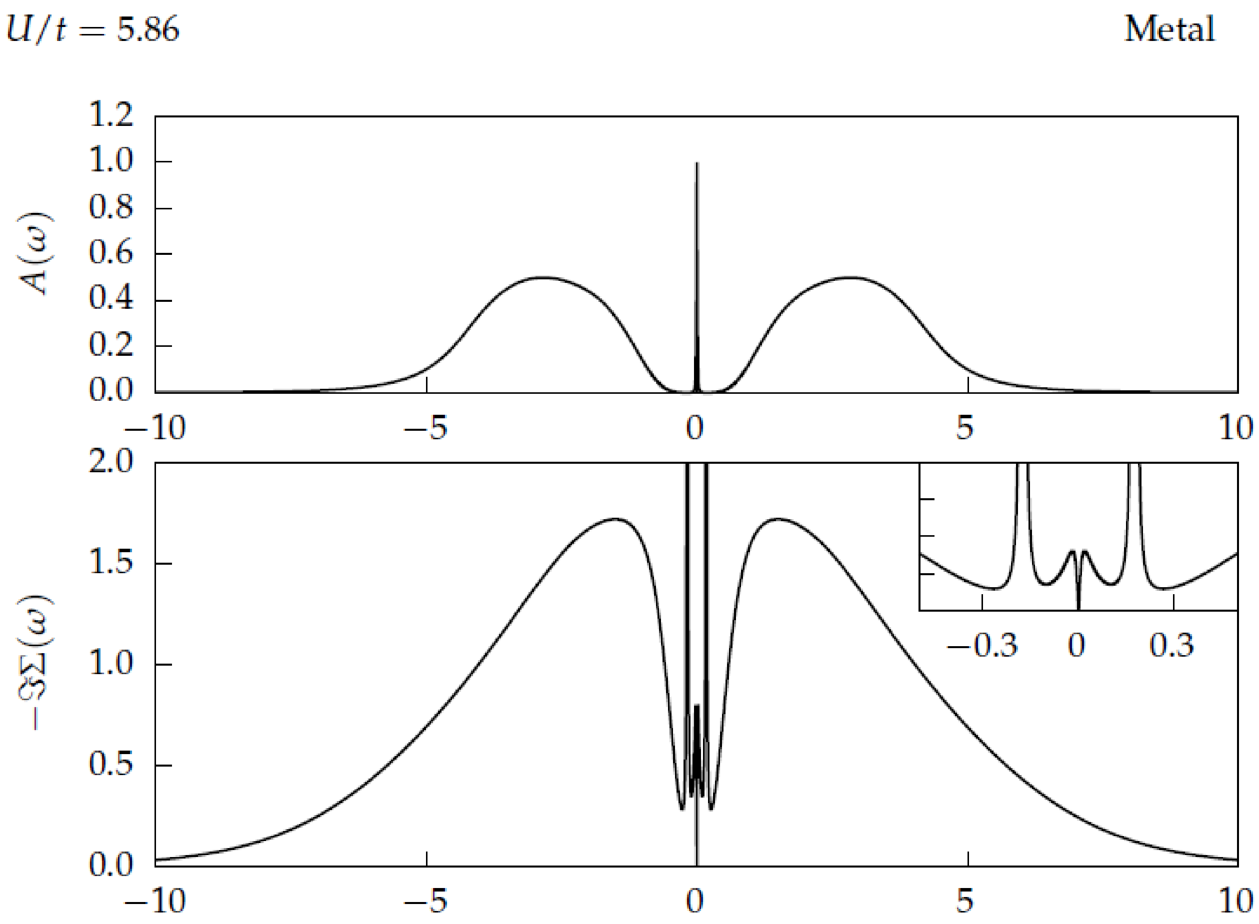
Structure of self-energy



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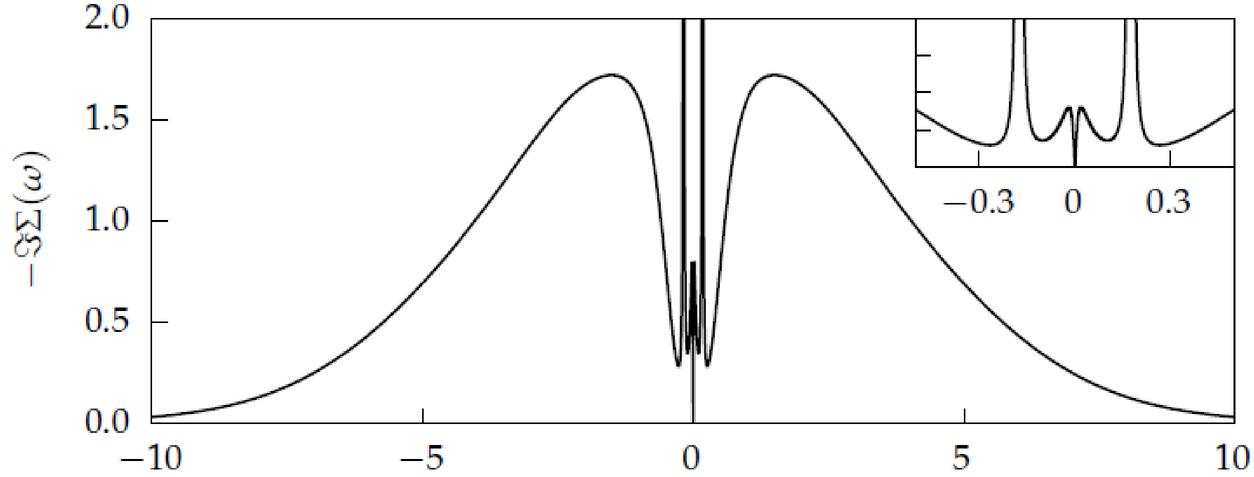
Structure of self-energy

Approaching transition from metallic side:

Self-energy develops double peak structure

As $U \rightarrow U_c^-$: peaks sharpen and coalesce

$$-t\,\mathrm{Im}\,\Sigma(\omega \rightarrow 0) \sim (\omega/Z)^2 \quad \text{with} \quad Z \rightarrow 0$$



Su-Schrieffer-Heeger (SSH) model

Paradigmatic model of a 1d topological insulator

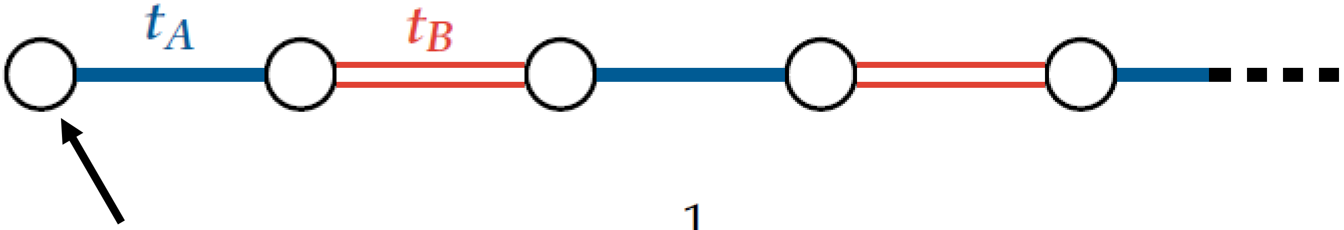
$$H_{\mathrm{SSH}} = \varepsilon \sum_{j=1}^{\infty} c_j^\dagger c_j + \left(t_A \sum_{j\ \mathrm{odd}} c_{j+1}^\dagger c_j + t_B \sum_{j\ \mathrm{even}} c_{j+1}^\dagger c_j + \mathrm{H.c.} \right)$$

Non-interacting!

Bulk is a band insulator with gap $\delta = |t_A - t_B|$

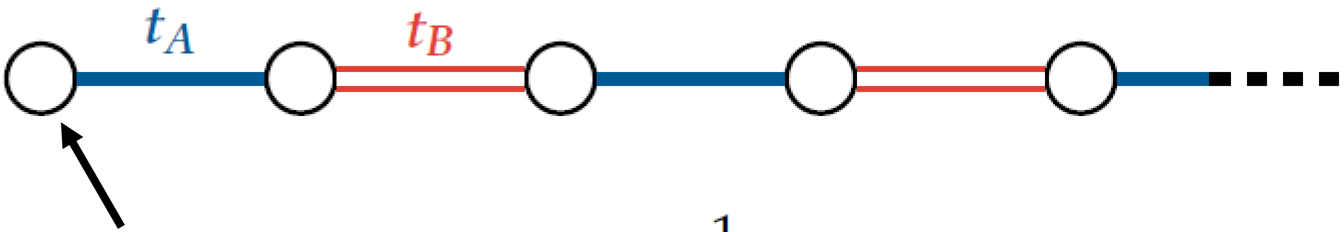
Phys. Rev. Lett. 42, 1698 (1979); Asbóth, Oroszlány, Pályi, Springer (2016)

SSH boundary Green's function



$$G_{1,1}(z) = \cfrac{1}{z-\varepsilon-\cfrac{t_A^2}{z-\varepsilon-\cfrac{t_B^2}{z-\varepsilon-\cfrac{t_A^2}{z-\varepsilon-\cfrac{t_B^2}{z-\varepsilon-\ddots}}}}}$$

SSH boundary Green's function



$$G_{1,1}(z) = \frac{1}{z - \varepsilon - \dfrac{t_A^2}{z - \varepsilon - t_B^2 G_{1,1}(z)}}$$

… solve for boundary GF

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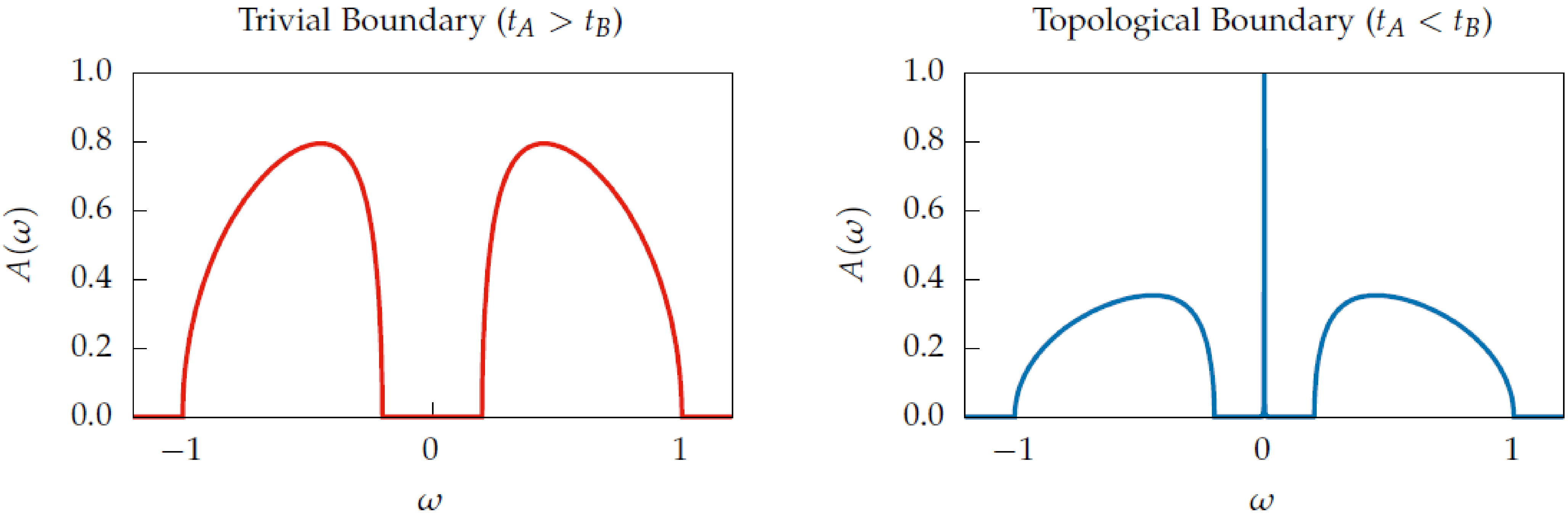
SSH boundary Green's function



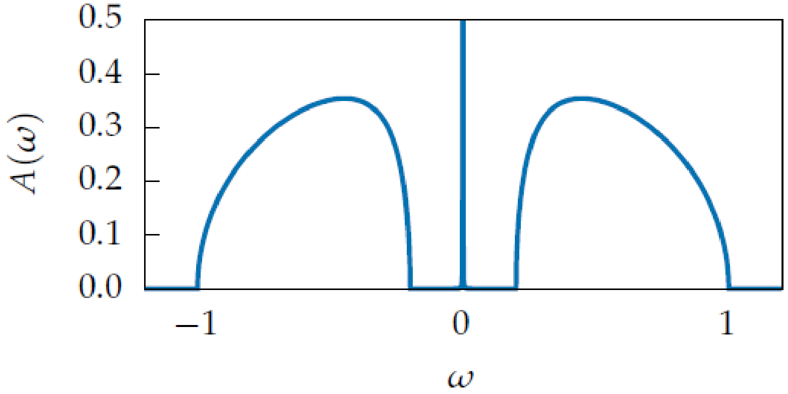
Boundary localized state

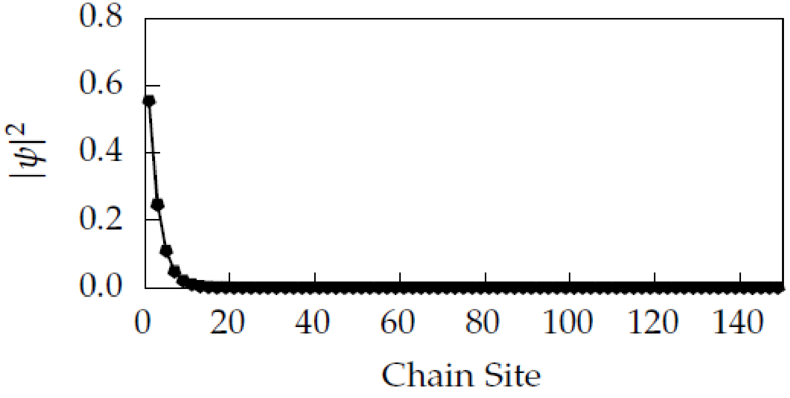
Transfer-matrix method:

zero-energy SSH eigenstate is exponentially localized on the boundary

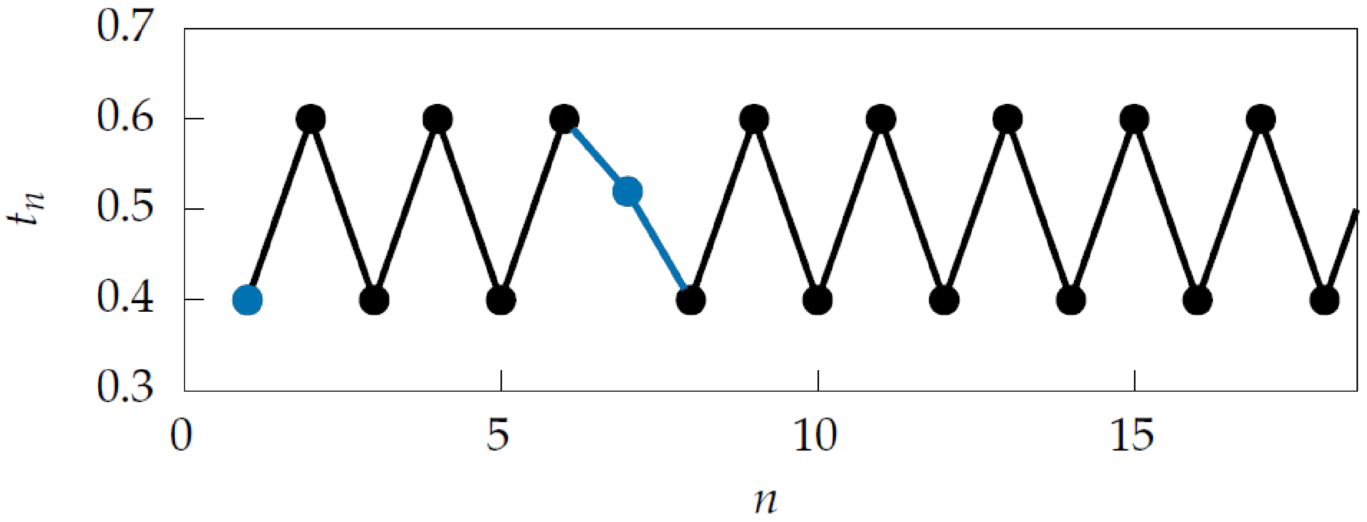
$$|\psi_0(2n-1)|^2 \sim \prod_{x=1}^{n} t_{2x-1}/t_{2x}$$
$$\sim \exp(-n/\xi) \text{ with } \xi \approx t/2\delta$$

Robust: requires only $t_{2n-1} < t_{2n}$





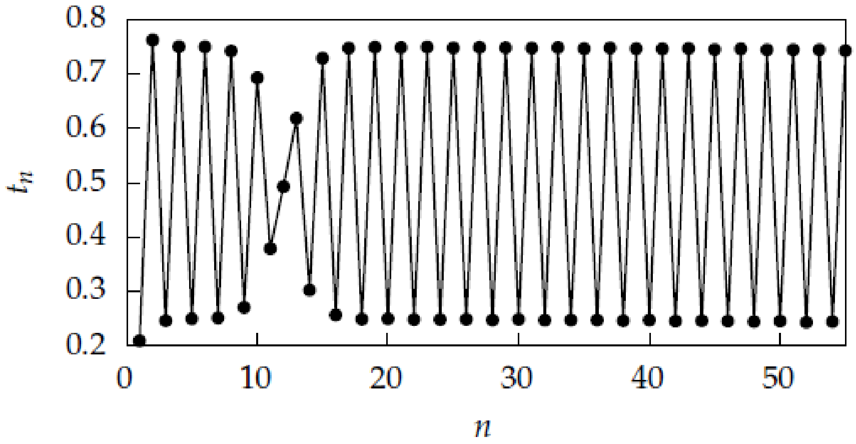
Domain Walls

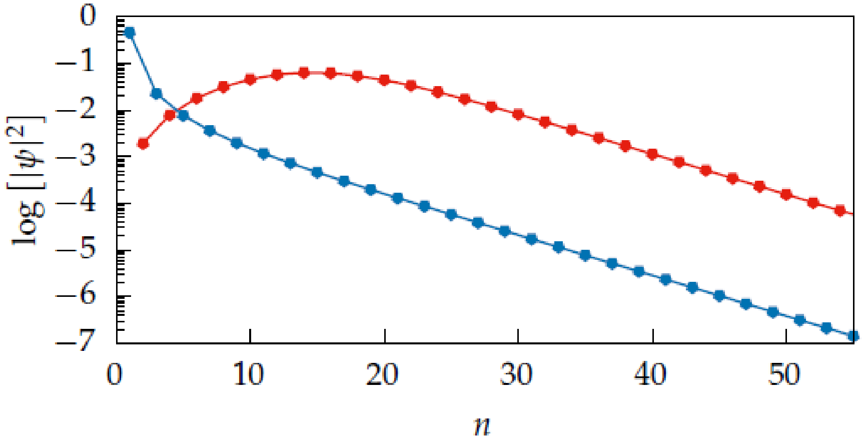


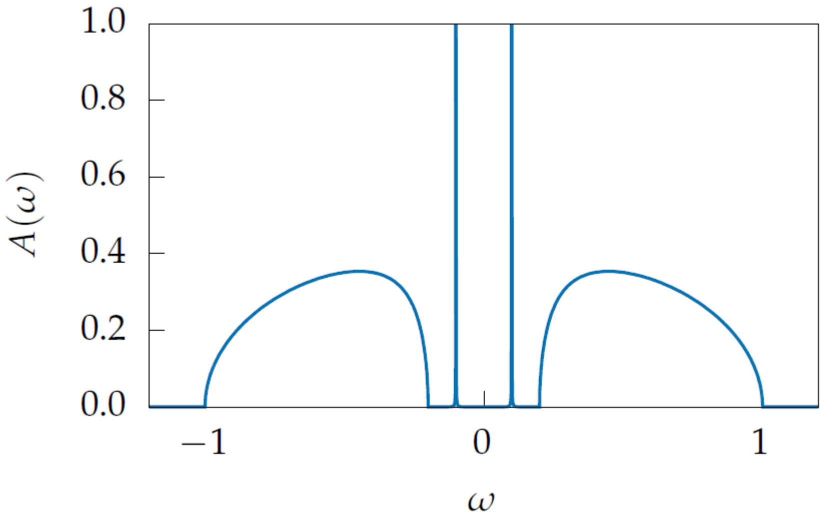
Localized states on the boundary and at domain walls

States hybridize and gap out: $\Delta\varepsilon \sim e^{-n_{\mathrm{dw}}/\xi}$

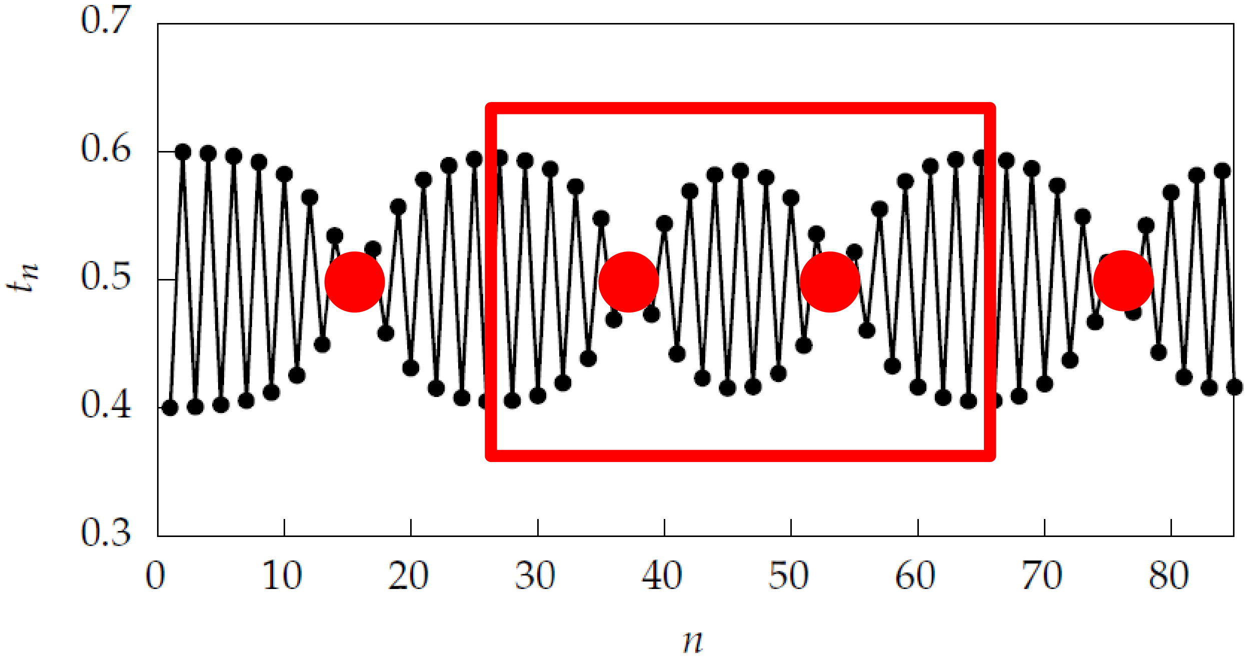
Domain Walls

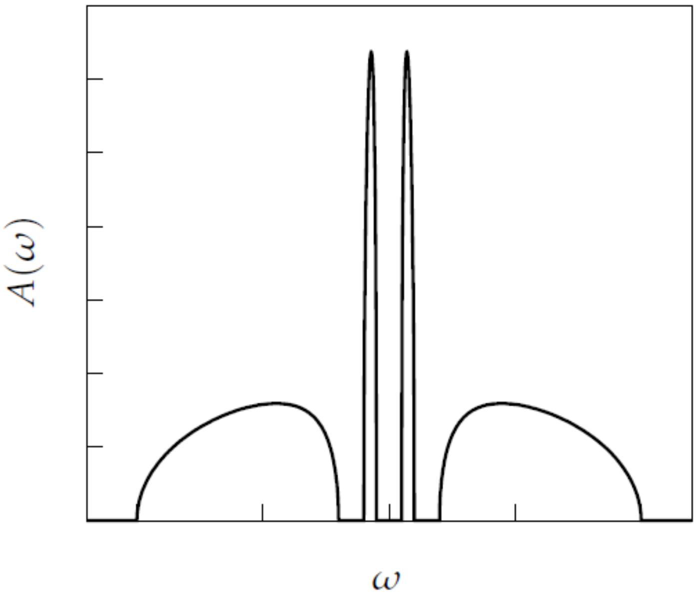




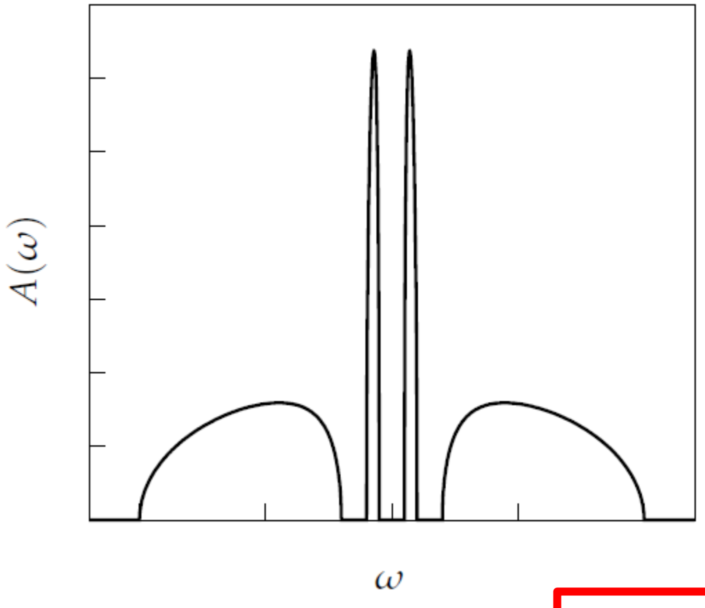


Bands of topological states





Moment Expansion method



Problem: What is the CFE of a composite spectrum

$$A(\omega) = \frac{1}{N}\sum_i w_i A_i(\omega)$$

given the CFE's of individual elements?

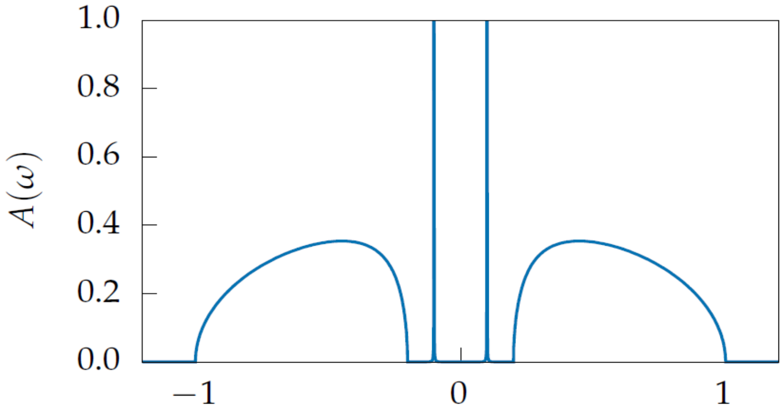
$$\mu_k = \frac{1}{N}\sum_i w_i \mu_{i,k} \quad \text{with} \quad \mu_{i,k} = \int d\omega\, \omega^k A_i(\omega)$$

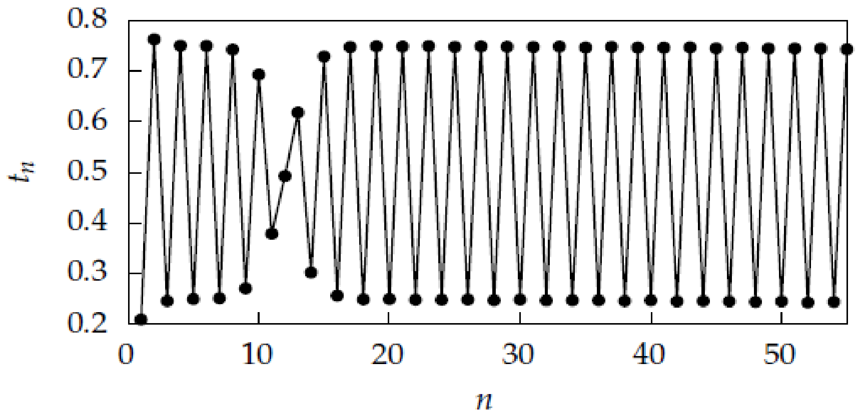
$$t_n^2 = X_n(n), \text{ where } X_k(n) = \frac{X_k(n-1)}{t_{n-1}^2} - \frac{X_{k-1}(n-2)}{t_{n-2}^2}$$

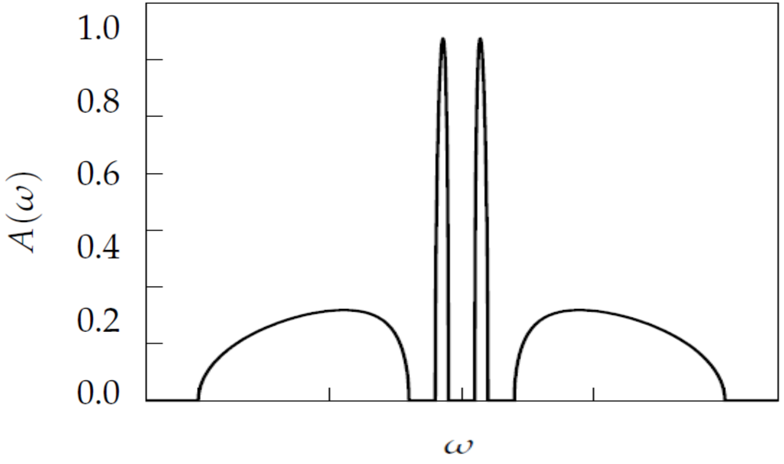
with $X_k(0) = \mu_{2k}$, $X_k(-1) = 0$, and $t_{-1}^2 = t_0^2 = 1$

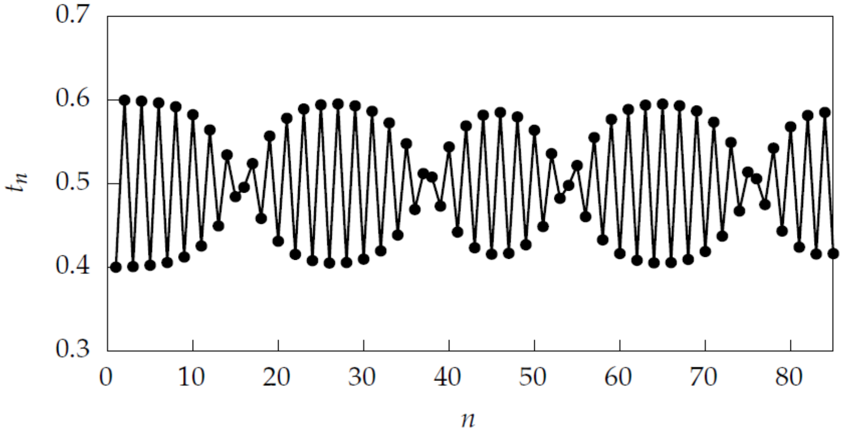
Vishwanath & Müller
Springer(1994)

Domain wall states





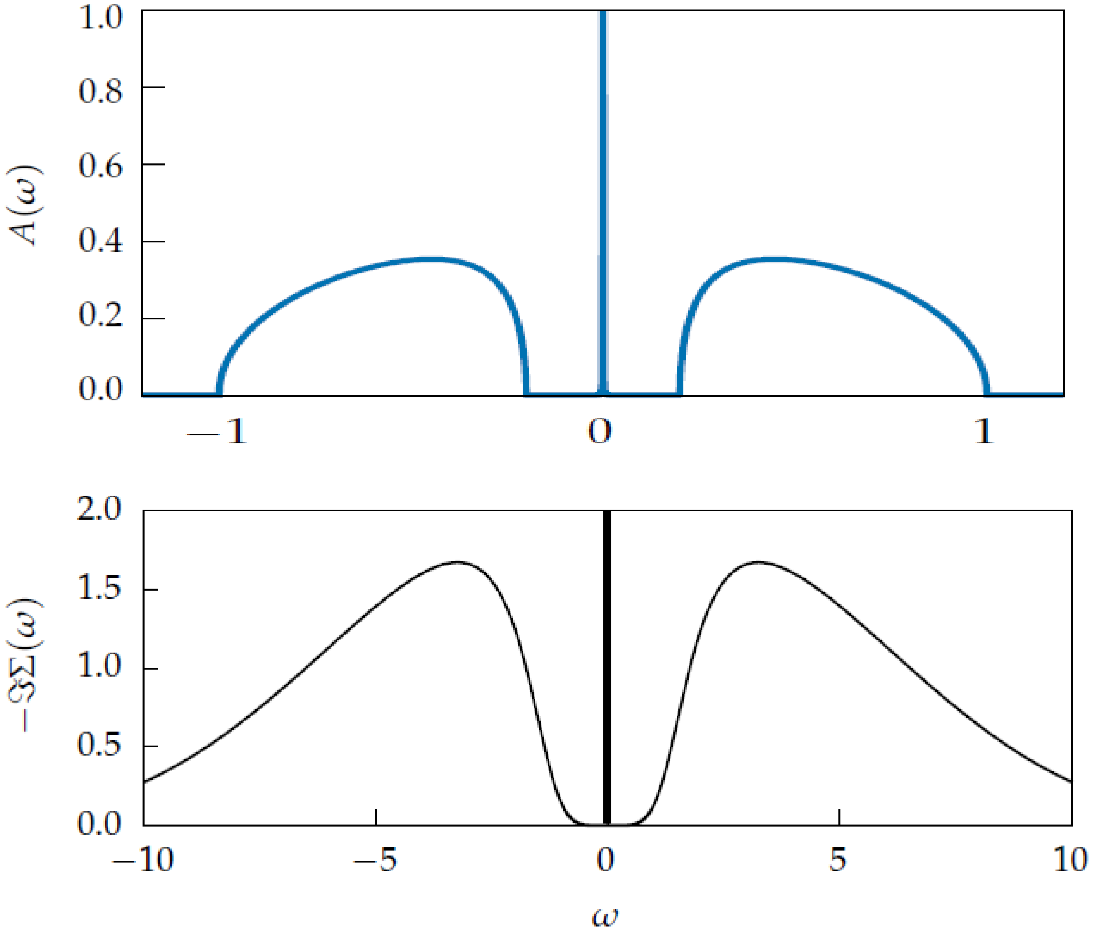




Topological phase?

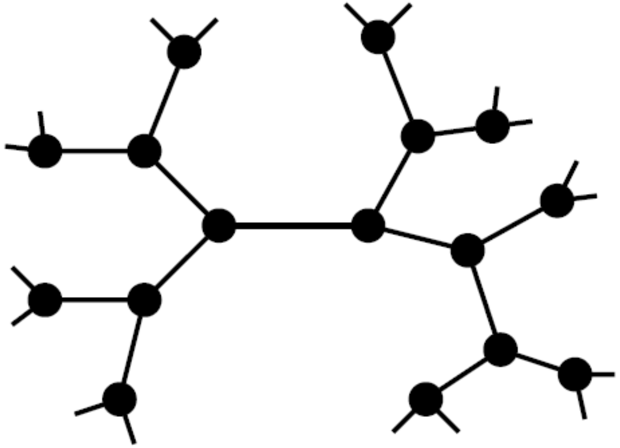
Topological SSH boundary GF

Mott insulator self-energy



Auxiliary field mapping

Scattering from e-e interactions can be reproduced **exactly** by coupling to auxiliary **non-interacting** dof's



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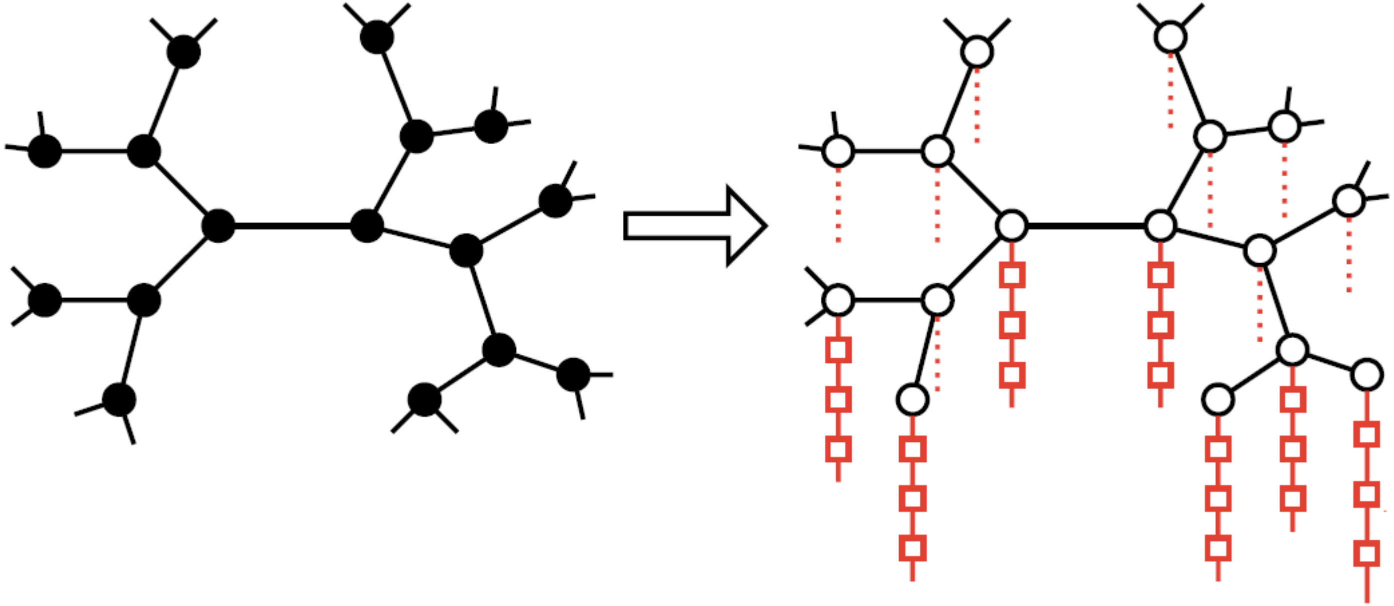

Auxiliary field mapping

Scattering from e-e interactions can be reproduced **exactly** by coupling to auxiliary **non-interacting** dof's

$$G_{latt}(\omega) = [\omega^+ - \epsilon - \Sigma_{latt}(\omega) - t^2 G_{latt}(\omega)]^{-1}$$

⇓

$$G_{latt}(\omega) = [\omega^+ - \epsilon - \Delta_0(\omega) - t^2 G_{latt}(\omega)]^{-1}$$

⇓

$$\Delta_0(\omega) = V^2 G_{aux}^0(\omega)$$

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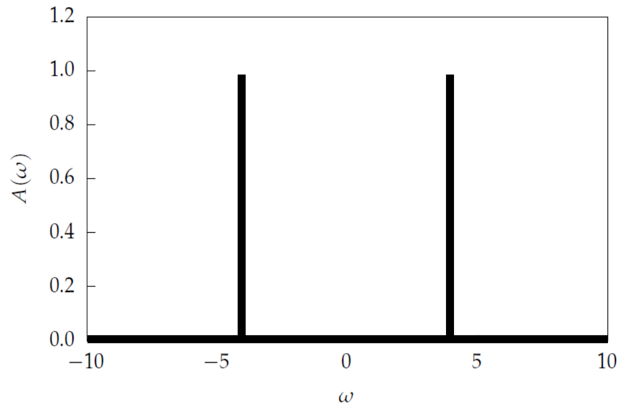
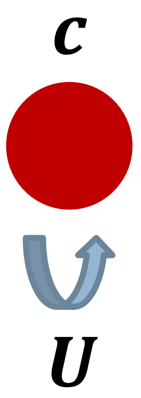
Example: Hubbard atom

$$H = U\left(c_\uparrow^\dagger c_\uparrow - \tfrac{1}{2}\right)\left(c_\downarrow^\dagger c_\downarrow - \tfrac{1}{2}\right)$$



$$G_{cc}(\omega) = \frac{1}{\omega^+ + U/2 - \Sigma(\omega)} \equiv \frac{1}{\omega^+ - \frac{(U/2)^2}{\omega^+}}$$

$$\Sigma(\omega) = \frac{U}{2} + \frac{(U/2)^2}{\omega^+} \equiv \Delta_0\,(\omega)$$



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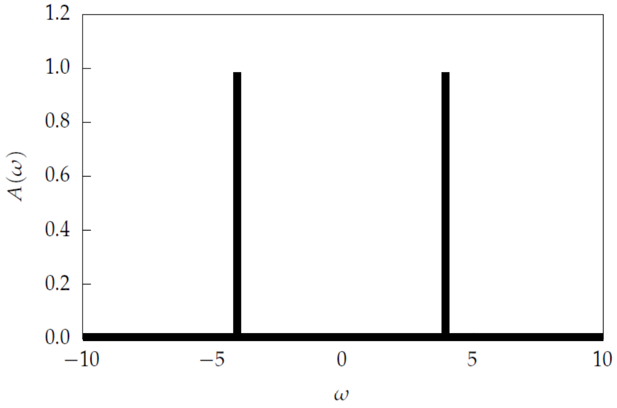

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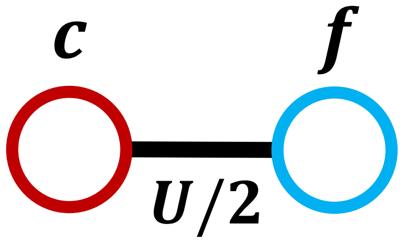


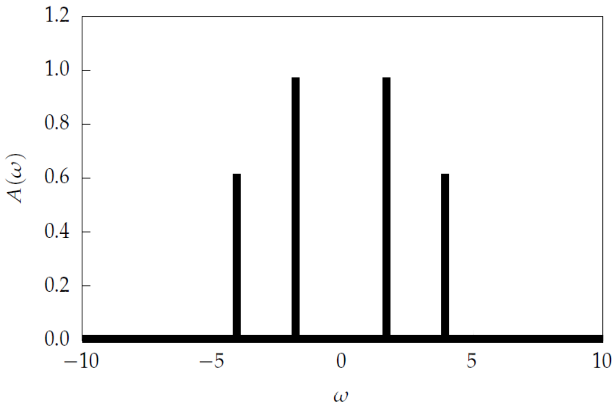
$$H_{map} = \frac{U}{2}\left(c^\dagger f + f^\dagger c\right)$$

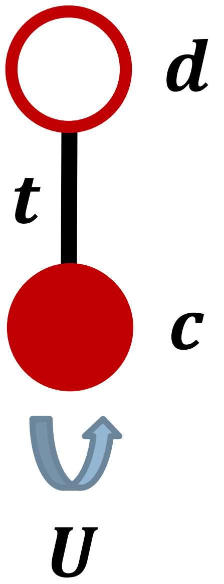
Example: Anderson dimer

$$H = U\left(c_\uparrow^\dagger c_\uparrow - \tfrac{1}{2}\right)\left(c_\downarrow^\dagger c_\downarrow - \tfrac{1}{2}\right) + t\sum_\sigma \left(c_\sigma^\dagger d_\sigma + d_\sigma^\dagger c_\sigma\right)$$

$$G_{cc}(\omega) = \frac{1}{\omega^+ + \frac{U}{2} - t^2/\omega^+ - \Sigma(\omega)}$$

$$\Sigma(\omega) = \frac{U}{2} + \frac{(U/2)^2}{\omega^+ - \frac{(3t)^2}{\omega^+}}$$



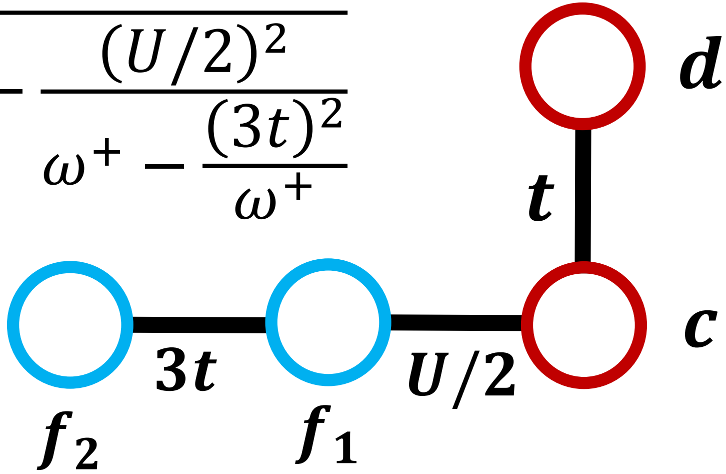


Example: Anderson dimer

$$H = U\left(c_\uparrow^\dagger c_\uparrow - \tfrac{1}{2}\right)\left(c_\downarrow^\dagger c_\downarrow - \tfrac{1}{2}\right) + t\sum_\sigma \left(c_\sigma^\dagger d_\sigma + d_\sigma^\dagger c_\sigma\right)$$

$$G_{cc}(\omega) = \frac{1}{\omega^+ + \frac{U}{2} - t^2/\omega^+ - \Sigma(\omega)} \equiv \frac{1}{\omega^+ - \frac{t^2}{\omega^+} - \frac{(U/2)^2}{\omega^+ - \frac{(3t)^2}{\omega^+}}}$$

$$\Sigma(\omega) = \frac{U}{2} + \frac{(U/2)^2}{\omega^+ - \frac{(3t)^2}{\omega^+}} \equiv \Delta_0(\omega)$$



$$H_{map} = t\left(c^\dagger d + d^\dagger c\right) + \frac{U}{2}\left(c^\dagger f_1 + f_1^\dagger c\right) + 3t\left(f_1^\dagger f_2 + f_2^\dagger f_1\right)$$

Non-linear canonical transformation

$$H = U\left(c_{\uparrow}^{\dagger}c_{\uparrow} - \tfrac{1}{2}\right)\left(c_{\downarrow}^{\dagger}c_{\downarrow} - \tfrac{1}{2}\right) + \epsilon_g g^{\dagger} g + \epsilon_f f^{\dagger} f$$

gauge degrees of freedom

Majorana representation:

$$c_{\uparrow}^{\dagger} = \frac{1}{2}(\gamma_1 + i\,\gamma_2) \qquad c_{\downarrow}^{\dagger} = \frac{1}{2}(\gamma_3 + i\,\gamma_4) \qquad g^{\dagger} = \frac{1}{2}(\gamma_5 + i\,\gamma_6) \qquad f^{\dagger} = \frac{1}{2}(\gamma_7 + i\,\gamma_8)$$

$$H = -\frac{U}{4}\gamma_1\gamma_2\gamma_3\gamma_4 - \frac{\epsilon_g}{2} i\,\gamma_5\gamma_6 - \frac{\epsilon_f}{2} i\,\gamma_7\gamma_8$$

Non-linear canonical transformation

$$H = -\frac{U}{4}\gamma_1\gamma_2\gamma_3\gamma_4 - \frac{\epsilon_g}{2} i\,\gamma_5\gamma_6 - \frac{\epsilon_f}{2} i\,\gamma_7\gamma_8$$

NLCT: $\mu_j = \hat{R}^\dagger \gamma_j \hat{R}$ with, $\hat{R} = exp\left[-i\frac{\theta}{2}\gamma_2\gamma_3\gamma_4\gamma_5\right]$

$$\mu_2 = -i\,\gamma_3\gamma_4\gamma_5$$
$$\mu_3 = +i\,\gamma_2\gamma_4\gamma_5$$
$$\mu_4 = -i\,\gamma_2\gamma_3\gamma_5$$
$$\mu_5 = +i\,\gamma_2\gamma_3\gamma_4$$

$$H = -\frac{U}{4} i\,\gamma_1\mu_5 - \frac{\epsilon_g}{2}\mu_2\mu_3\mu_4\gamma_6 - \frac{\epsilon_f}{2} i\,\gamma_7\gamma_8$$

Bazzanella, Nilsson, arXiv:1405.5176

Non-linear canonical transformation

$$H = -\frac{U}{4} i\,\gamma_1\mu_5 - \frac{\epsilon_g}{2}\mu_2\mu_3\mu_4\gamma_6 - \frac{\epsilon_f}{2} i\,\gamma_7\gamma_8$$

Gauge choice: $\epsilon_g = 0$ and $\epsilon_f = \frac{U}{2}$

$$H = -\frac{U}{4} i(\gamma_1\mu_5 + \gamma_7\gamma_8)$$

Refermionization: $\alpha^\dagger = \frac{1}{2}(\gamma_1 + i\,\gamma_8)$ $\beta^\dagger = \frac{1}{2}(\gamma_7 + i\,\gamma_5)$

$$H = \frac{U}{2}\left(\alpha^\dagger\beta + \beta^\dagger\alpha\right)$$

⇒ $G_{cc(\omega)} = G_{\alpha\alpha}(\omega)$

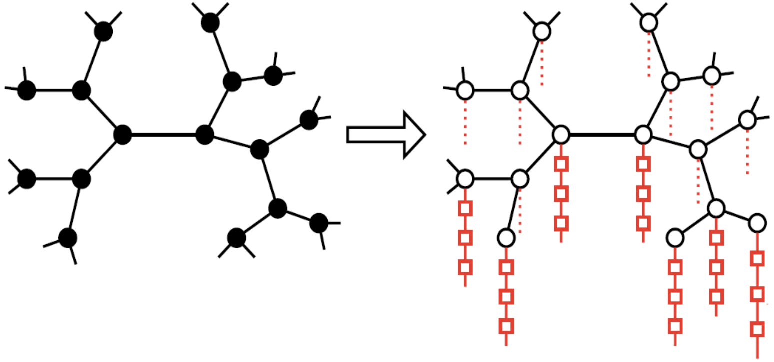
Auxiliary field mapping

Scattering from e-e interactions can be reproduced **exactly** by coupling to auxiliary **non-interacting** dof's

$$H_{\text{int}} \to H_{\text{aux}} + H_{\text{hyb}}$$

$$H_{\text{aux}} = \sum_{i,\sigma} \sum_{n=1}^{\infty} t_n (f^{\dagger}_{i\sigma,n} f_{i\sigma,n+1} + \text{H.c.})$$

$$H_{\text{hyb}} = V \sum_{i,\sigma} (c^{\dagger}_{i\sigma} f_{i\sigma,1} + f^{\dagger}_{i\sigma,1} c_{i\sigma})$$



Auxiliary field mapping

Our strategy for the Hubbard model:

find the self-energy using DMFT-NRG
map to auxiliary 1d chains
analyze the properties of the auxiliary system

$$\Sigma(\omega) \to \Delta_0(\omega) = V^2 G^0_{aux}(\omega) = \cfrac{V^2}{z - \cfrac{t_1^2}{z - \cfrac{t_2^2}{z - \cfrac{t_3^2}{\ddots}}}}$$

Continued Fraction Expansion

Auxiliary field mapping

Continued Fraction Expansion of self-energy:

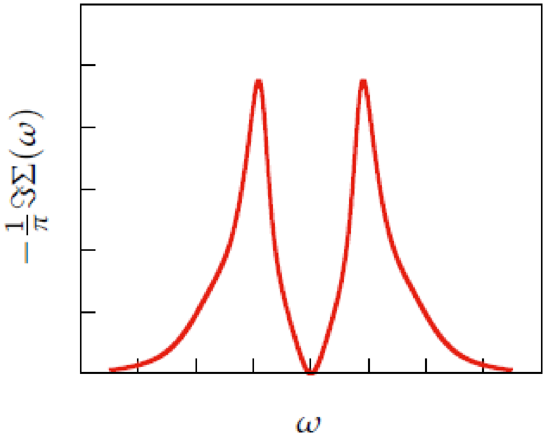
$$\Sigma(\omega) \to \Delta_0(\omega)$$

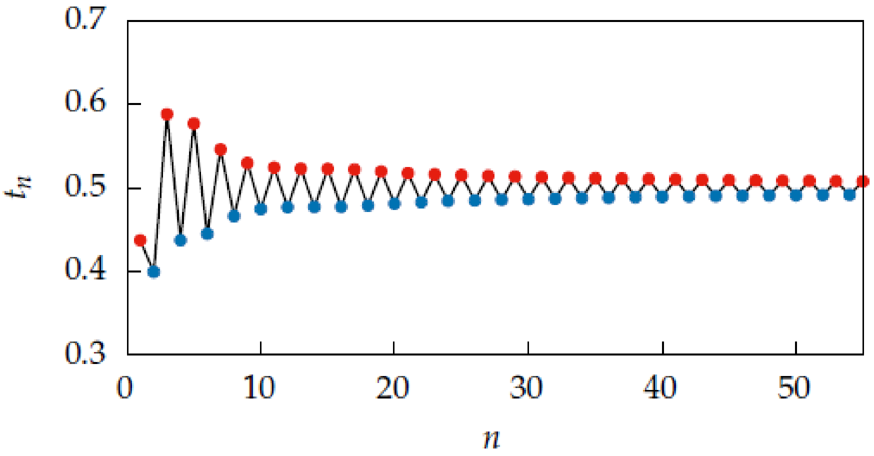
$$\Delta_n(\omega) = t_n^2/[\omega^+ - \Delta_{n+1}(\omega)]$$

$$t_n^2 = -\tfrac{1}{\pi}\mathrm{Im}\int d\omega\, \Delta_n(\omega)$$

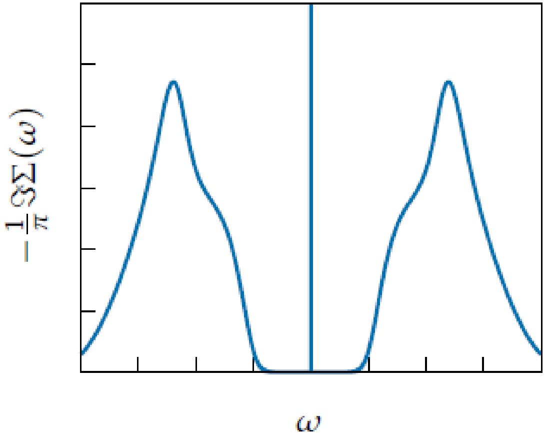
Auxiliary field mapping

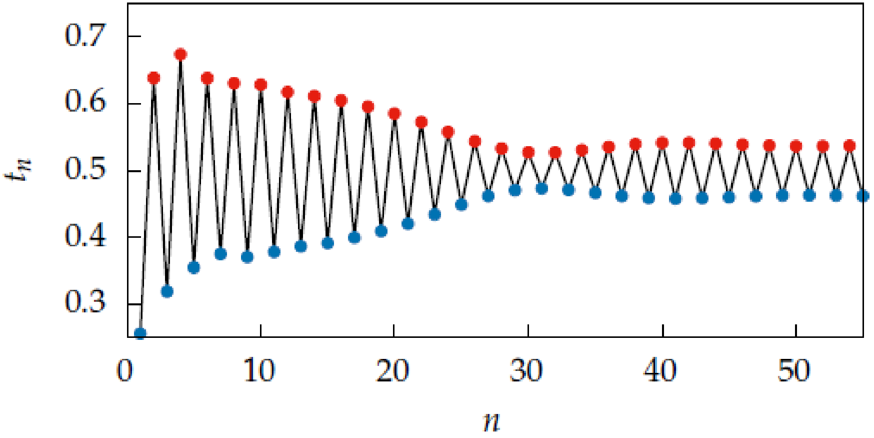
Metal:





Insulator:





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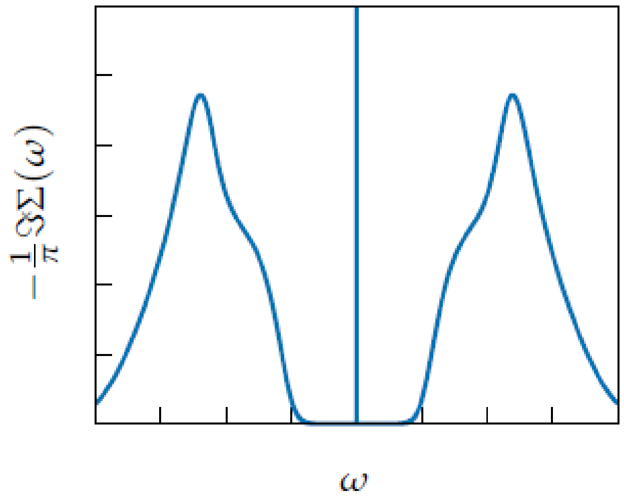
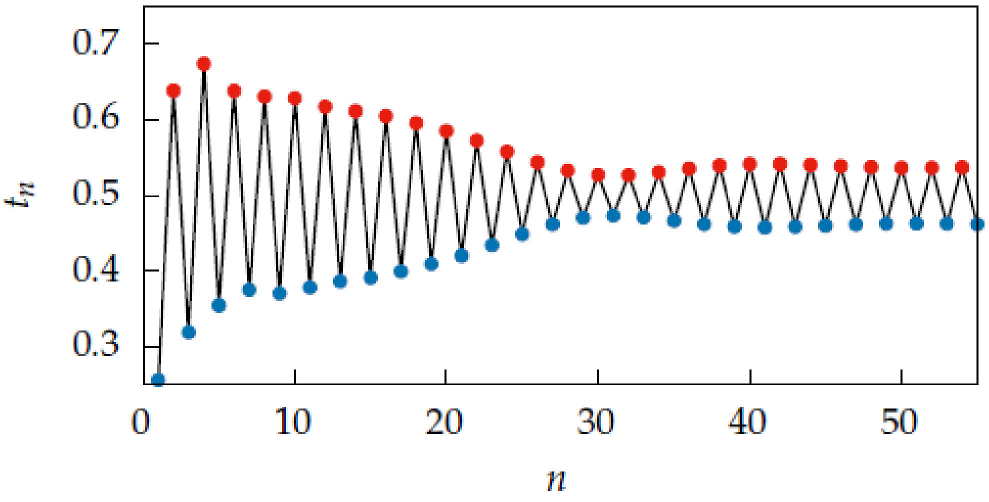
Mott insulator

SSH model in the topological phase with hopping perturbations

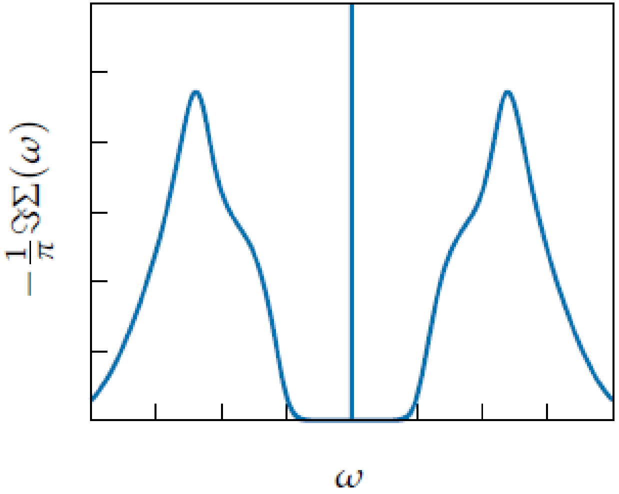


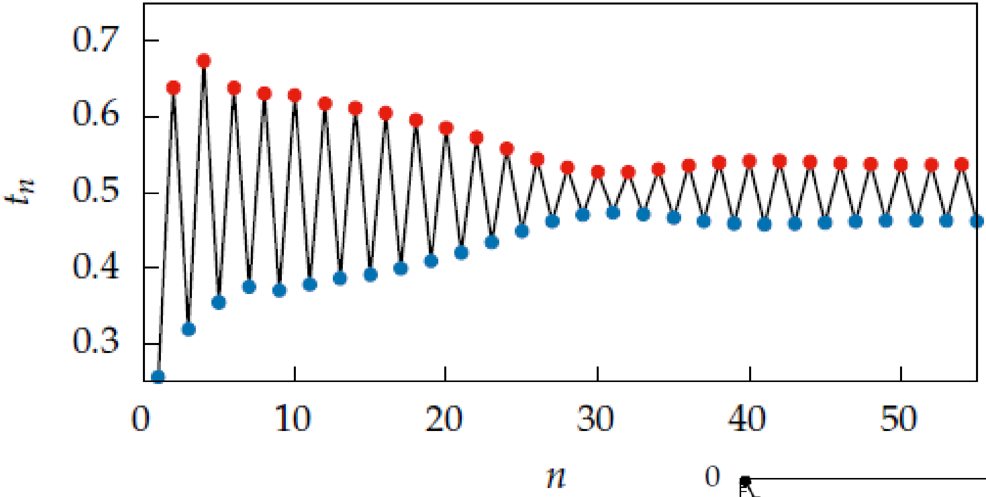


$$t_n \overset{n\delta/D \gg 1}{\sim} \frac{1}{2}[D + (-1)^n \delta]$$

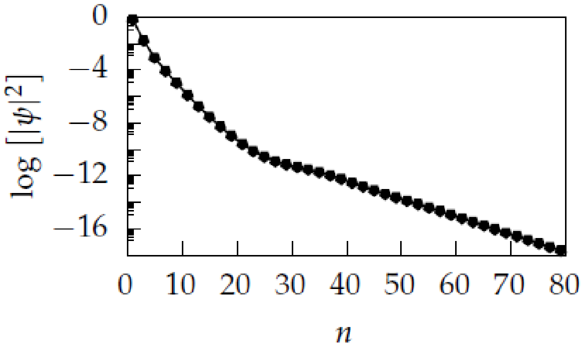
Mott insulator

SSH model in the topological phase with hopping perturbations



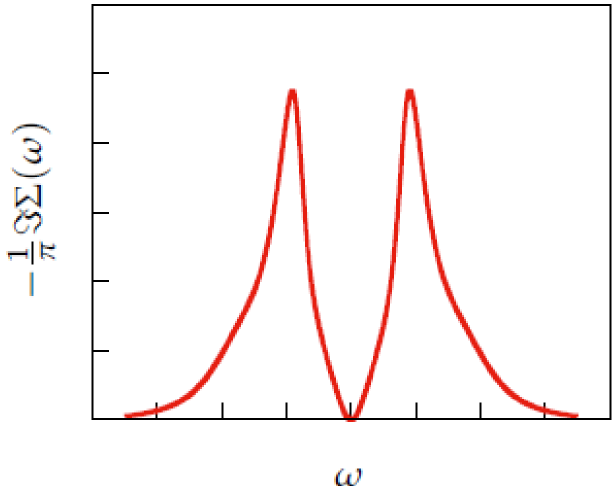


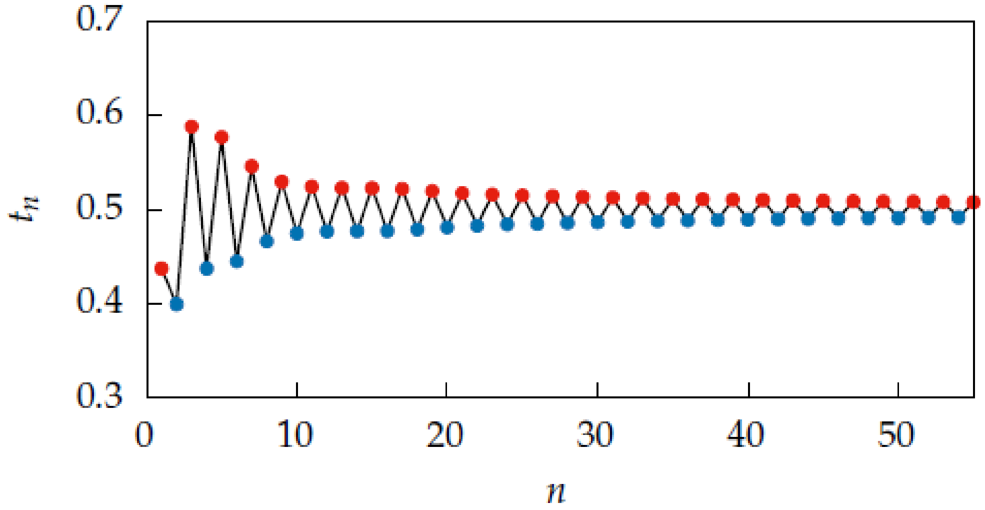
Mott pole corresponds to boundary localized state:



Metal (fermi liquid)

Generalized (pseudogap) SSH model in the trivial phase



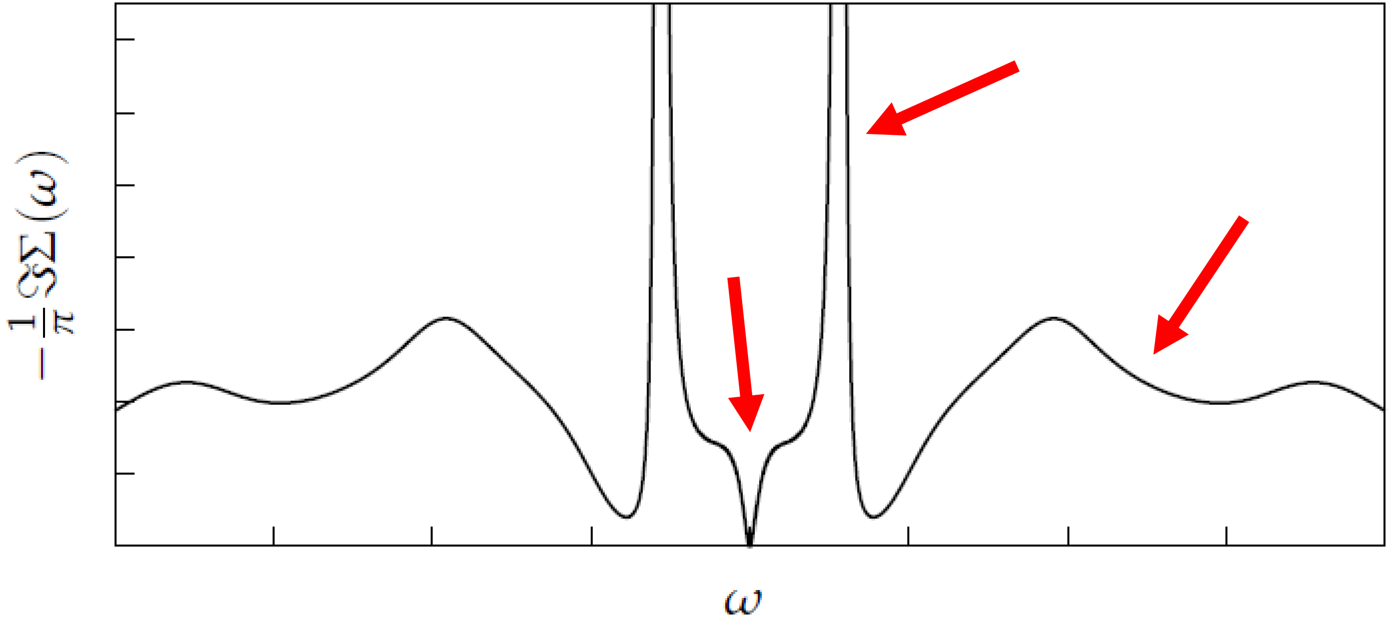


$$t_n^2 \overset{nZ \gg 1}{\sim} \frac{D^2}{4}\left[1 - \frac{r}{n+d}(-1)^n\right]$$

Topological phase transition?

No bulk gap closing across Mott transition!

Double-peak structure in self-energy near the transition!



(i) Hubbard bands

(ii) Double peak

(iii) Pseudogap

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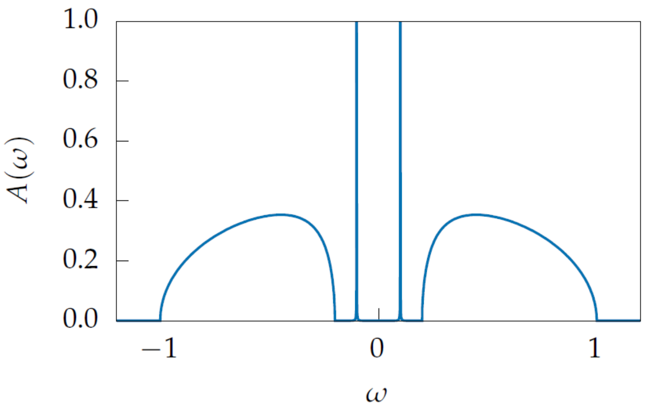
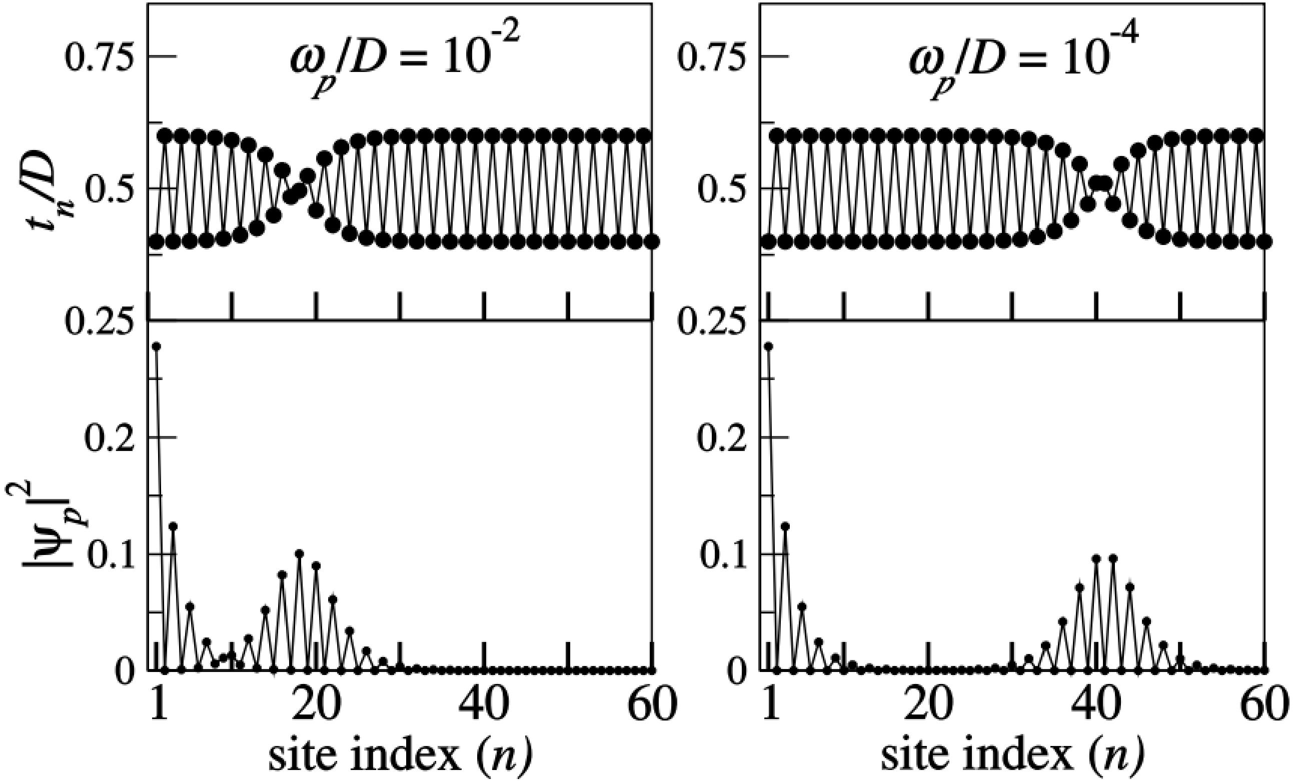
Topological phase transition?

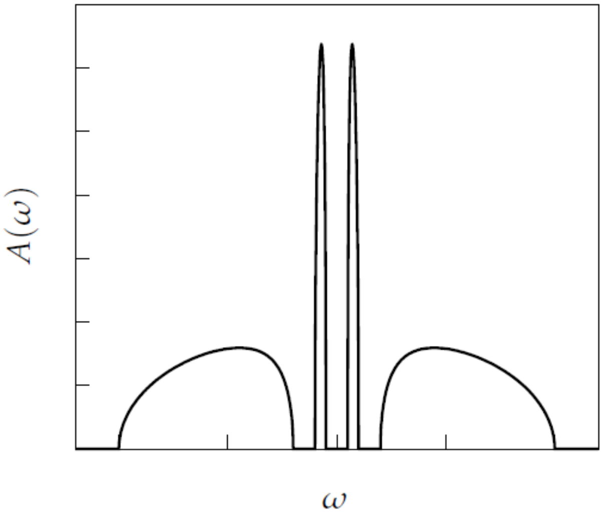
Double peaks coalesce across transition

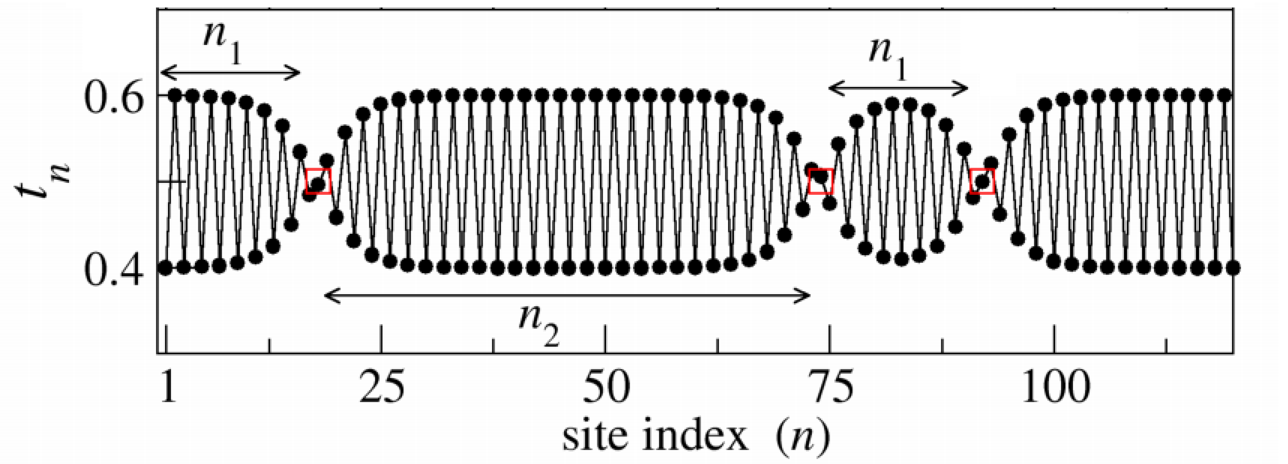




Topological phase transition?

Peaks not poles!





Low-energy pseudogap gives additional 1/n envelope

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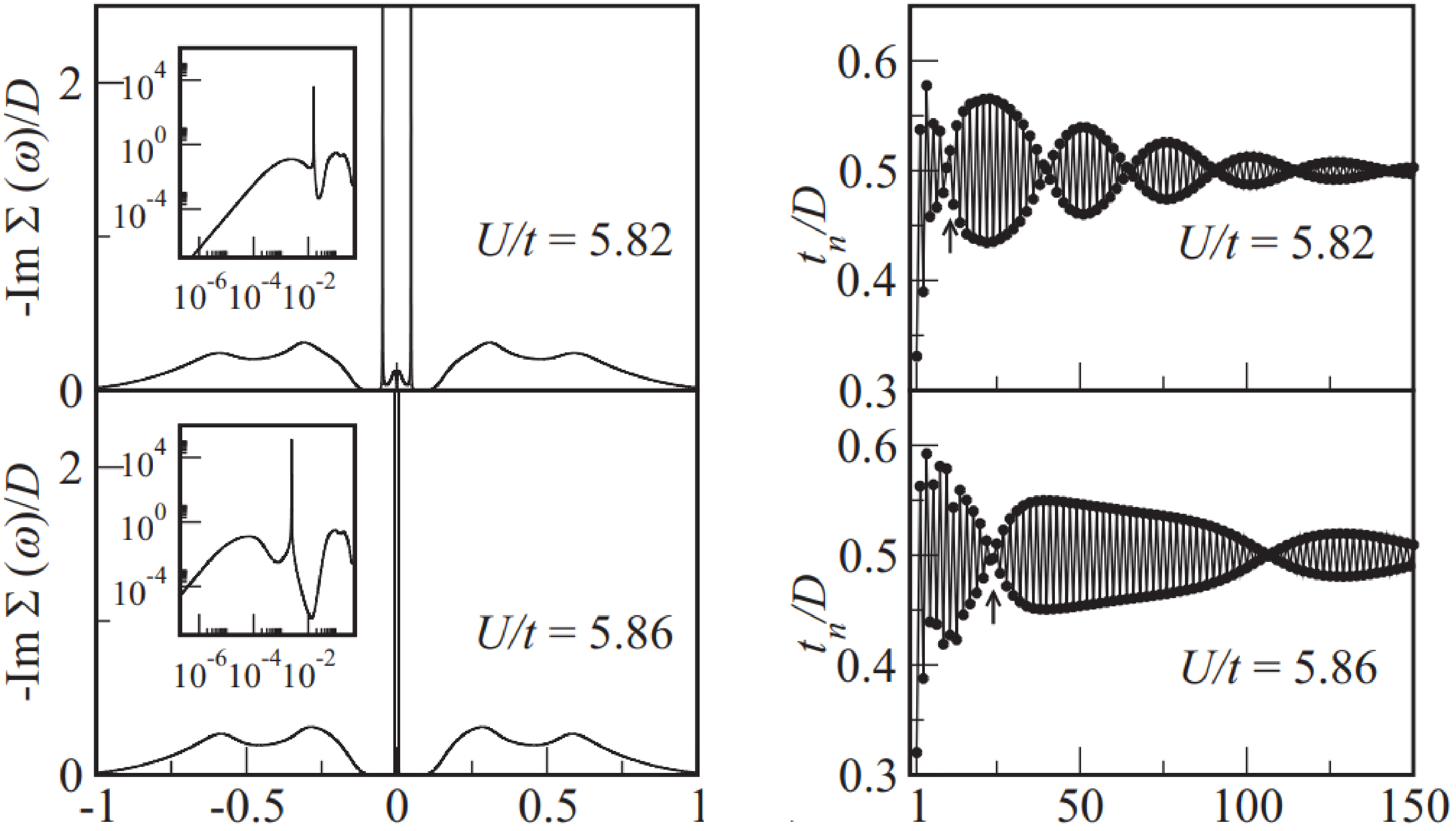
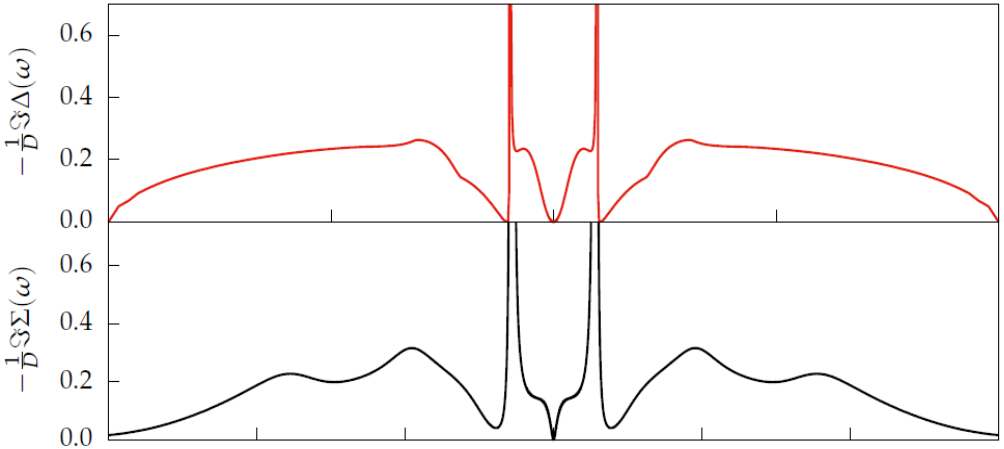
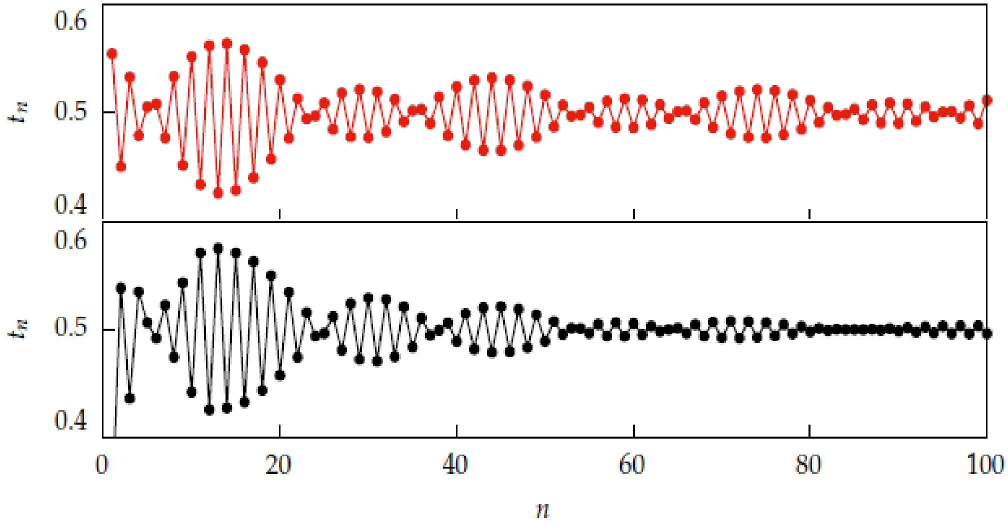
Topological phase transition



Toy model for the transition

$$t_n^2 = \frac{D^2}{4}\left[1 - \frac{2}{n+d}(-1)^n\right] \times \left[1 - \beta\cos\left(\frac{2\pi n}{\lambda} + \phi\right)\right]$$





Topological integral invariant?

Luttinger integral

$$I_{\mathrm{L}} = \frac{2}{\pi}\Im\int_{-\infty}^{0} \mathrm{d}\omega\ G(\omega)\frac{\mathrm{d}\Sigma(\omega)}{\mathrm{d}\omega}$$

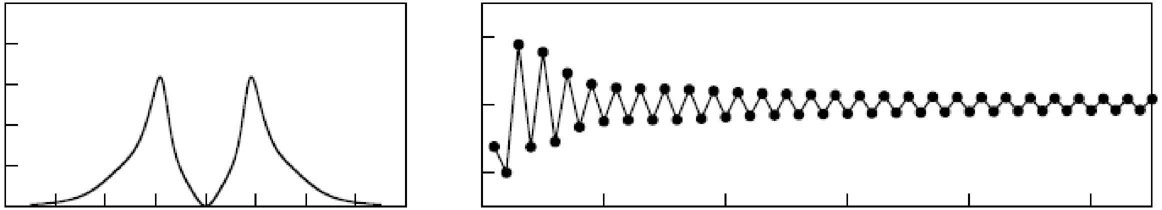
$$= \begin{cases} 0 & \forall U < U_c \quad \text{Fermi liquid} \\ 1 & \forall U > U_c \quad \text{Mott insulator} \end{cases}$$

- I_L plays the role of the topological invariant
  - Finite (*integer*) value in topological phase
  - Zero in trivial phase
  - Similar form to Volovik-Essin-Gurarie invariant
- I_L dependent upon Σ
  - Topology is encoded in Σ

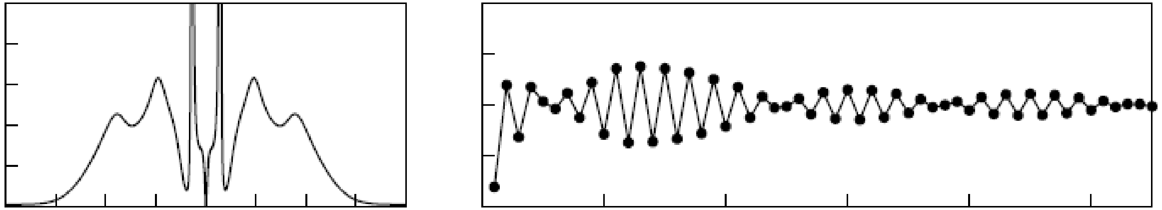
D. E. Logan and M. R. Galpin, J. Phys.: Condens. Matter **28**, 025601 (2015)

Summary

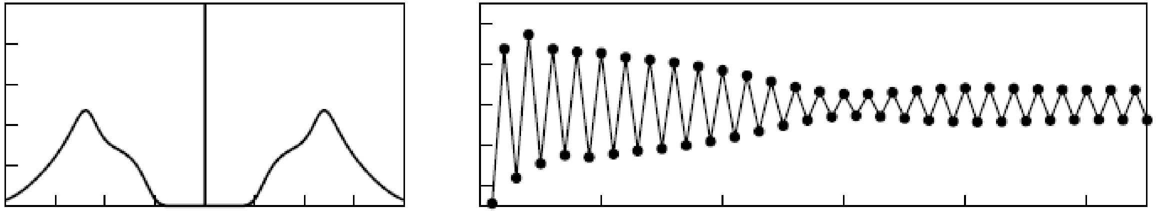
Self-energy of Hubbard model mapped to auxiliary non-interacting chain of generalized SSH type



Metallic phase:
"Pseudogap" SSH chain in trivial phase. No localized states.



Near Mott transition:
Domain wall formation and dissociation



Mott insulator:
SSH chain in the topological phase with a single boundary localized Mott pole state

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Outlook

Multi-orbital Hubbard model or cluster DMFT: coupled SSH chains

Momentum-dependent self-energy: D-dim physical lattice gives (D+1)-dim auxiliary lattice

Non-equilibrium dynamics: Melting Mott insulator via interaction quench

Superconducting phase: Auxiliary Kitaev chain with Majoranas???