Optical Conductivity of Strongly Correlated Electron Systems in High Dimensions

N. Blümer

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Outline

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Introduction

Definition of the Optical Conductivity $\sigma(\omega)$

Linear response of time-invariant (unperturbed) system on electric field $\boldsymbol{E}(\boldsymbol{r}, t)$:

$$J_\alpha(\boldsymbol{r}, t) = \sum_\beta \int \mathrm{d}\boldsymbol{r}' \int_{-\infty}^{t} \mathrm{d}t'\, \sigma_{\alpha\beta}(\boldsymbol{r}, \boldsymbol{r}', t - t')\, E_\beta(\boldsymbol{r}', t')$$

Homogeneous system, long-wavelength limit $\boldsymbol{q} \to 0$:

$$J_\alpha(\omega) = \sum_\beta \sigma_{\alpha\beta}(\omega)\, E_\beta(\omega)$$

Optical conductivity $\sigma_{\alpha\beta}(\omega)$:

- symmetric complex tensor
- retarded function: analytic in upper half plane (Kramers-Kronig)

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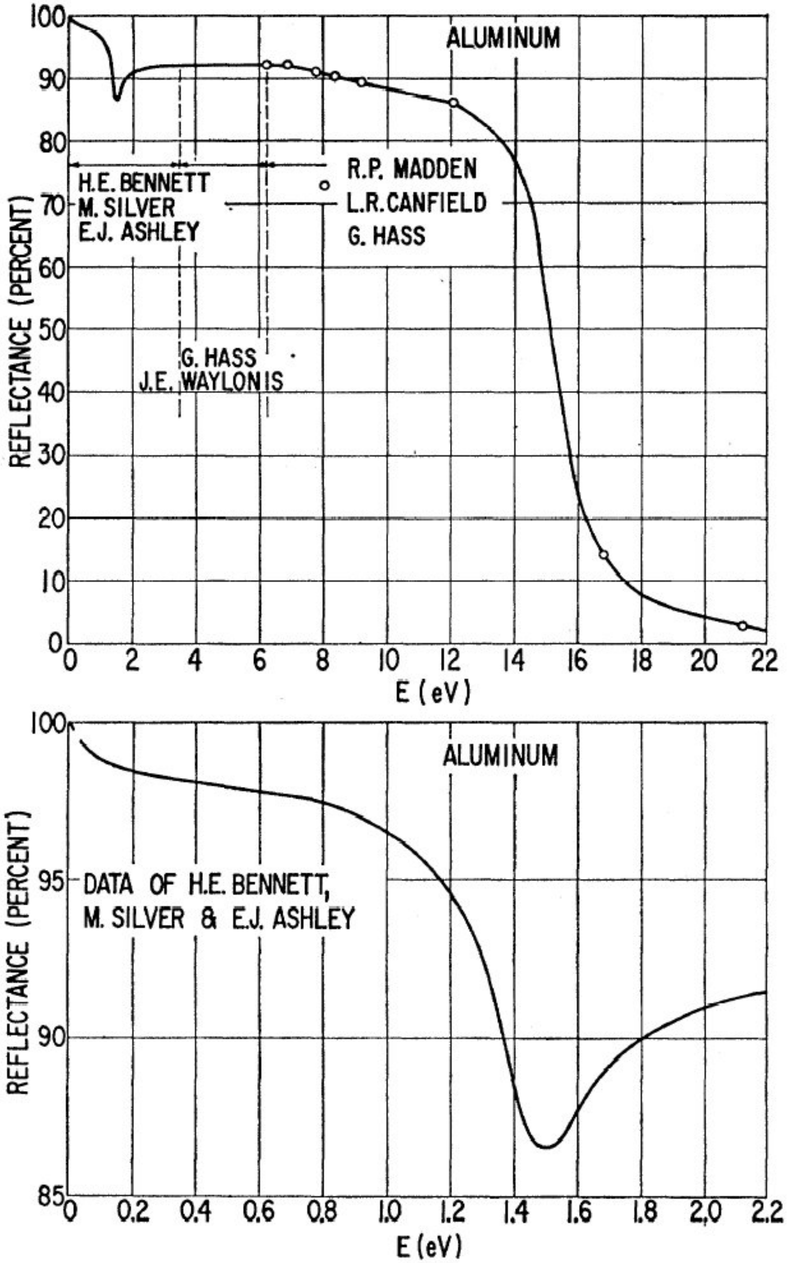
Connection with Reflectivity and Experiment

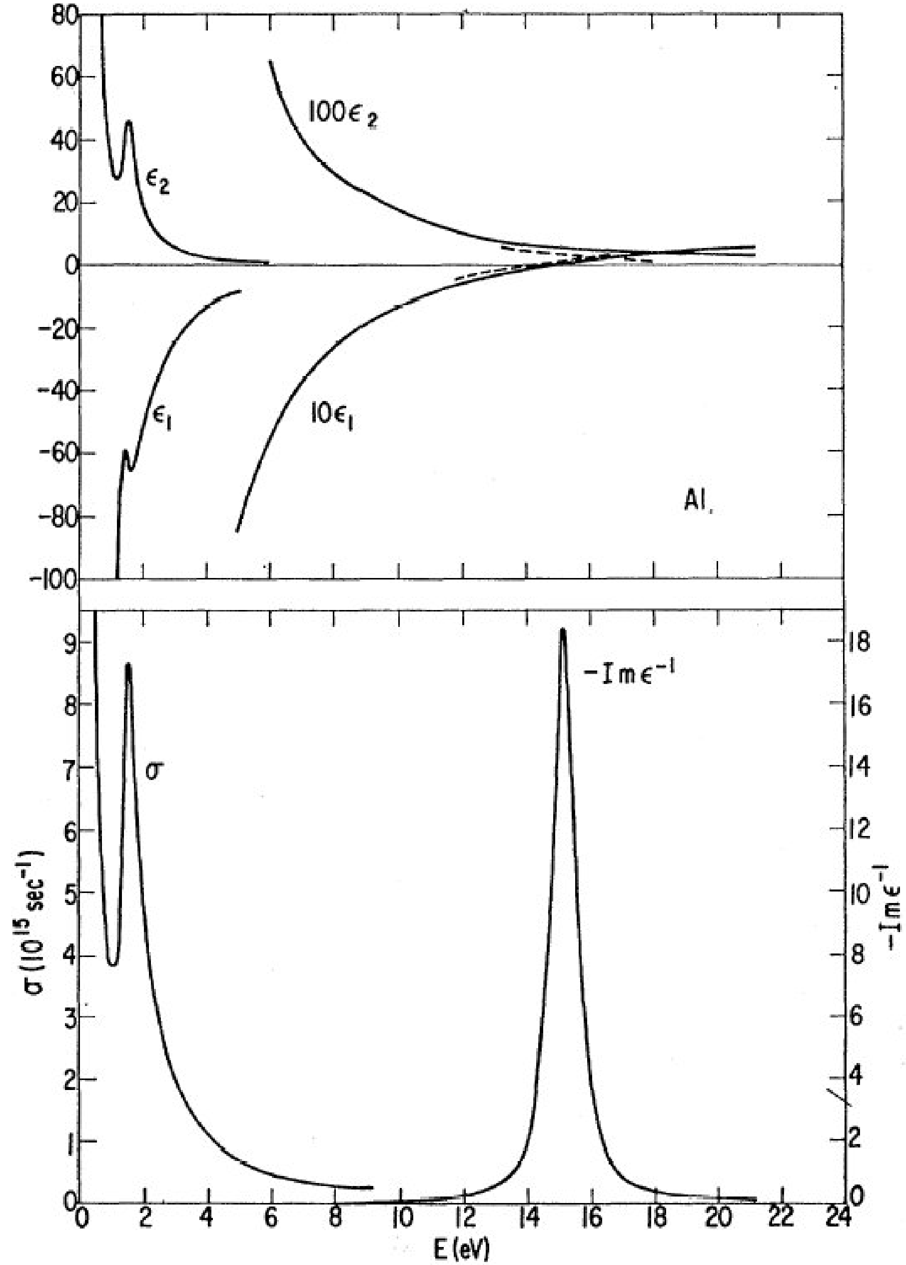
Dielectric function $\epsilon(\omega) = 1 + \frac{4\pi i}{\omega} \sigma(\omega)$ and $\kappa(\omega) \equiv \sqrt{\epsilon(\omega)}$ also analytic

Reflectivity (for normal incidence): $r(\omega) = \left| \frac{1-\kappa(\omega)}{1+\kappa(\omega)} \right|^2$

Determine $\sigma(\omega)$ from
- specular reflectivity $r(\omega)$ in large frequency range (use Kramers-Kronig)
- reflectivity at varying angles
- transmission experiments (absorption and phase)

Example: good metal Al [H. Ehrenreich, H. R. Philipp, and B. Segall, Phys. Rev. **132**, 1918 (1963)]





The f-sum rules

bounded absorption spectrum:

$$\epsilon(\omega) \xrightarrow{\omega\to\infty} 1 - \frac{\omega_\mathrm{p}^2}{\omega^2}$$

$$\frac{2}{\pi}\int_0^\infty d\omega\, \omega\, \mathrm{Im}\, \epsilon(\omega) = \omega_\mathrm{p}^2$$

$$\Longrightarrow \left\{ \begin{array}{lcl} \int_0^\infty \mathrm{d}\omega\, \mathrm{Re}\, \sigma(\omega) & = & \frac{\omega_\mathrm{p}^2}{8} \\ \int_0^\infty \mathrm{d}\omega\, \omega\, \mathrm{Im}\, \kappa(\omega) & = & \frac{\pi}{4}\omega_\mathrm{p}^2 \\ \int_0^\infty \mathrm{d}\omega\, \omega\, \mathrm{Im}\, \frac{-1}{\epsilon(\omega)} & = & \frac{\pi}{2}\omega_\mathrm{p}^2 \end{array} \right.$$

Optical f-sum rule

The f-sum rules

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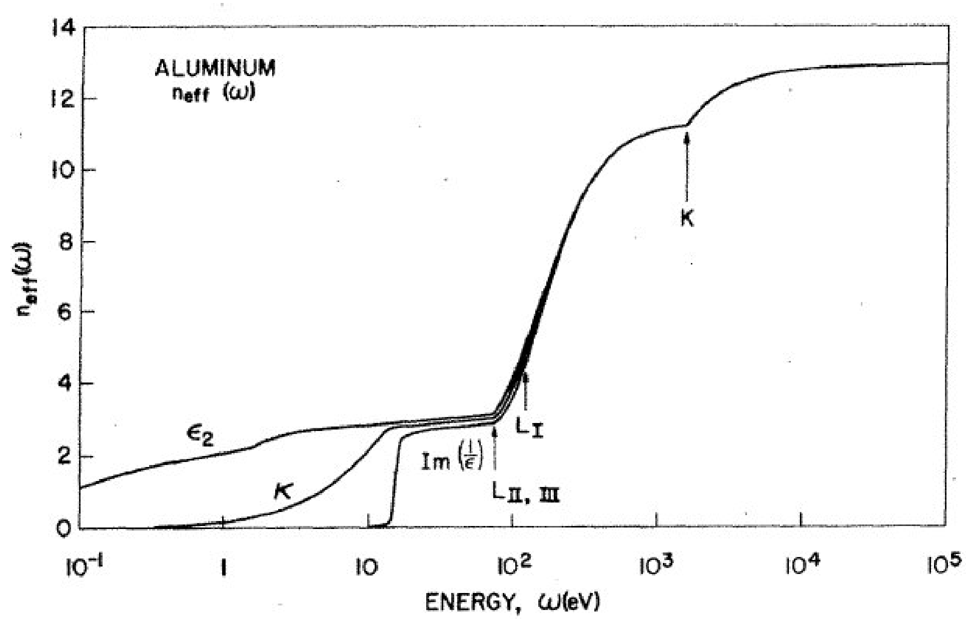
Full universal f-sum rule: $\omega_\text{p}^2 = \frac{4\pi n e^2}{m}$

frequency cutoff $\omega_\text{c} \longrightarrow$ partial sum rules

$$\omega_{\text{p, valence}}^2 = \frac{4\pi n_\text{v}\, e^2}{m^*} \equiv \frac{4\pi e^2}{m} n_\text{eff}(\omega_\text{c})$$

non-universal!



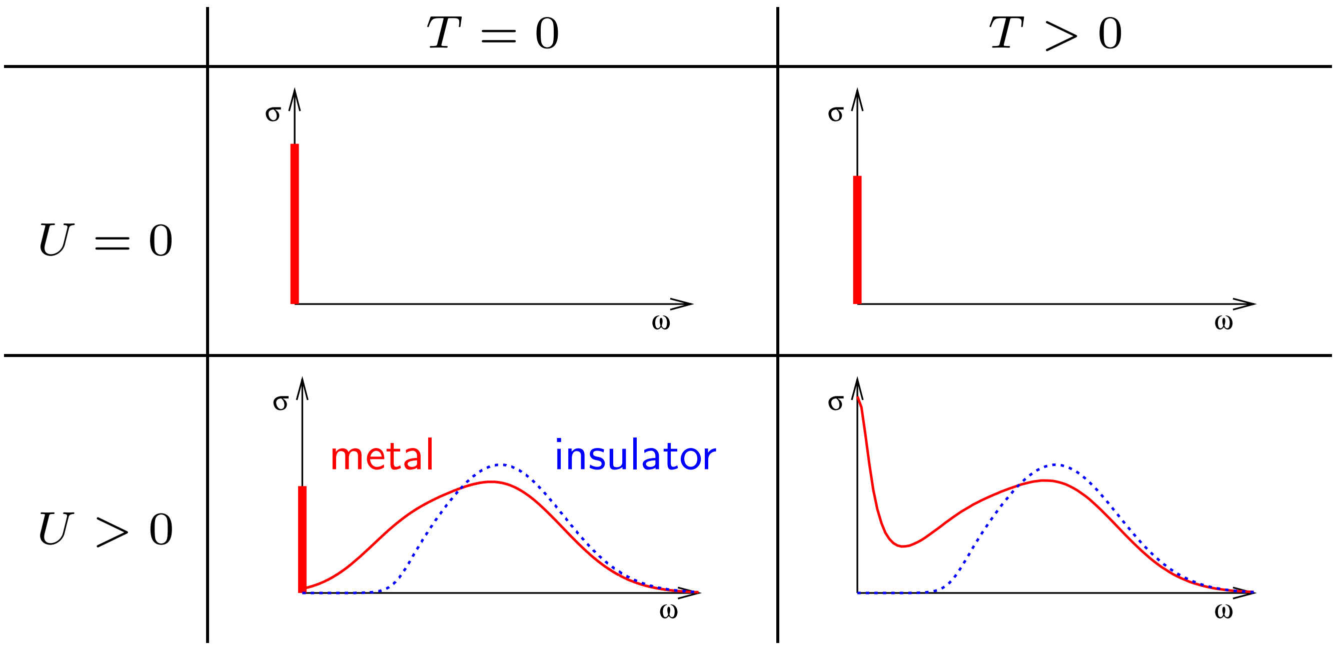
[D. Y. Smith and E. Shiles, Phys. Rev. B **17**, 4689 (1978)]

Lattice Model

Unperturbed lattice Hamiltonian (here single-band Hubbard model):

$$\hat{H} = \hat{H}_0 + \hat{H}_{\text{int}} = \sum_{\sigma} \sum_{i,j} t_{ij} (\hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} + \hat{c}^\dagger_{j\sigma} \hat{c}_{i\sigma}) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

For regular Bravais lattice and translation invariant hopping: $\hat{H}_0 = \sum_{\boldsymbol{k},\sigma} \epsilon_{\boldsymbol{k}} \, \hat{n}_{\boldsymbol{k},\sigma}$

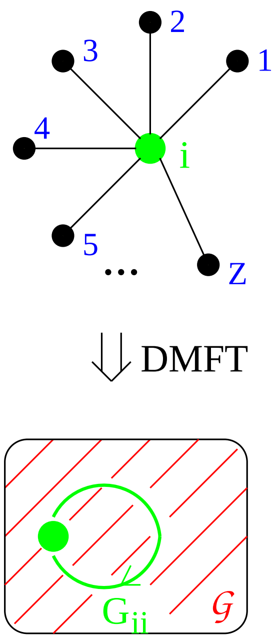


nontrivial $\sigma(\omega)$
due to correlations

Non-universal optical f-sum rule, depends on U and T!

For nearest-neighbor hopping on hypercubic lattice: $\int_0^\infty d\omega \, \sigma(\omega) = -\frac{\pi}{2} \frac{e^2 a^2}{V \hbar^2} \frac{1}{d} \langle \hat{H}_0 \rangle$

Dynamical Mean Field Theory (DMFT)

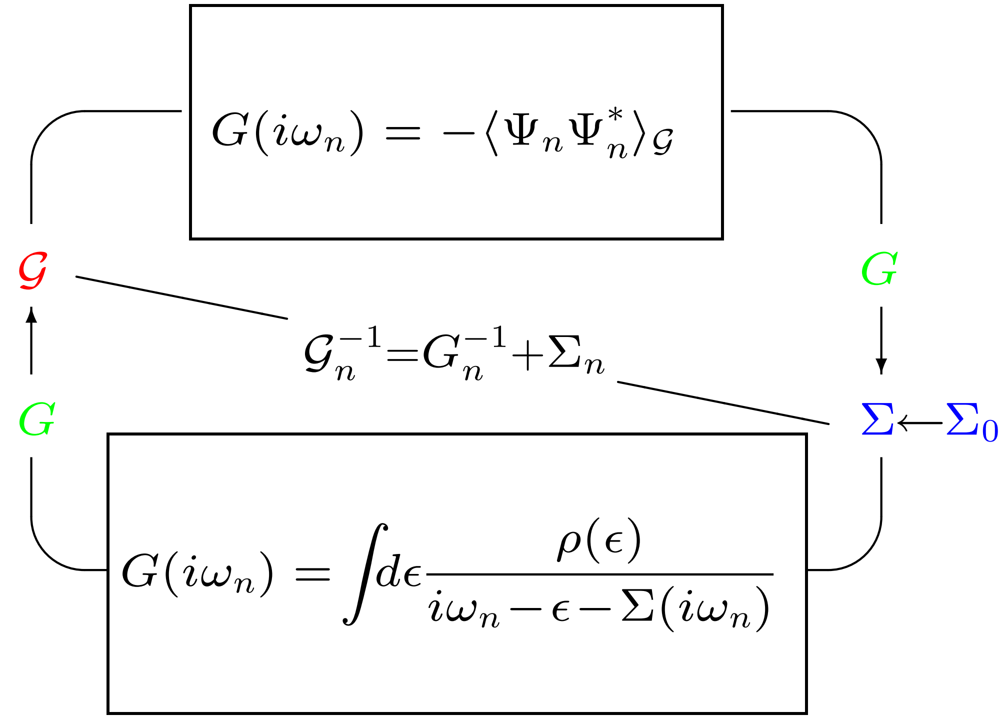


scaling of hopping matrix elements $t \propto 1/\sqrt{Z}$

mapping of lattice problem onto impurity model
$+$ self consistency condition

local self energy $\Sigma(\omega)$

exact for $Z \to \infty$



[W. Metzner and D. Vollhardt, Phys. Rev. Lett. **62**, 324 (1989)]

[A. Georges et. al, Rev. Mod. Phys. **68**, 13 (1996)]

Lattice enters only via noninteracting density of states (DOS)

nonperturbative approach, suitable for studies at intermediate / strong coupling:

- ferromagnetism, metamagnetism, orbital ordering
- metal insulator transitions (MIT)
- improvement on band-structure DFT calculations: LDA+DMFT

Density of States (DOS) in High Dimensions

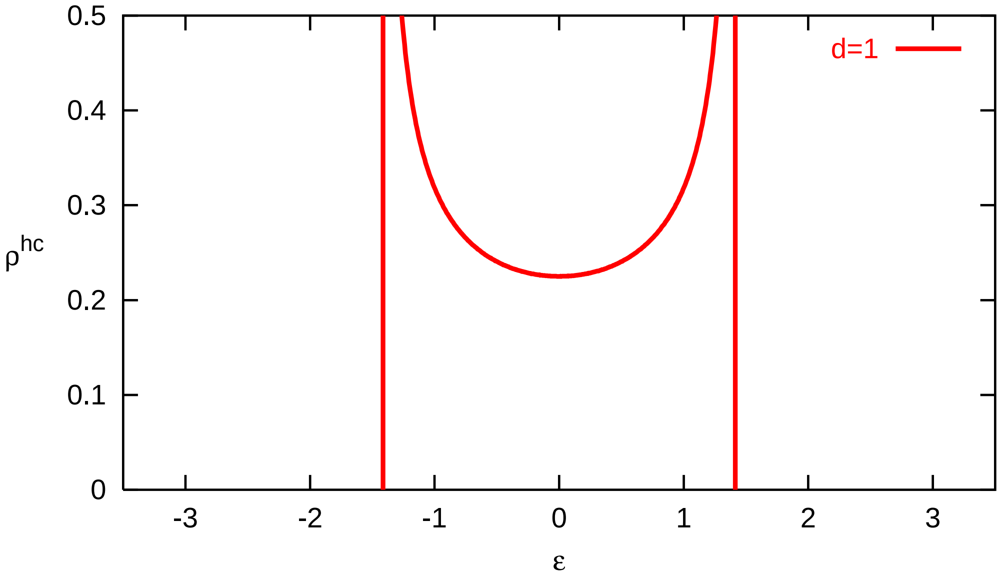
For uniform nearest neighbor (NN) hopping on a hypercubic (hc) lattice:

$$\epsilon_{\boldsymbol{k}}^{\text{hc}} = -2t \sum_{\alpha=1}^{d} \cos(k_\alpha)$$

Unit variance of DOS for scaling $t = t^*/\sqrt{2d}$

for $d \to \infty$: band edges at $\pm\sqrt{2d}$ diverge

$$\rho^{\text{hc}}(\epsilon) = \frac{1}{\sqrt{2\pi}t^*} e^{-\epsilon^2/(2t^{*2})}$$



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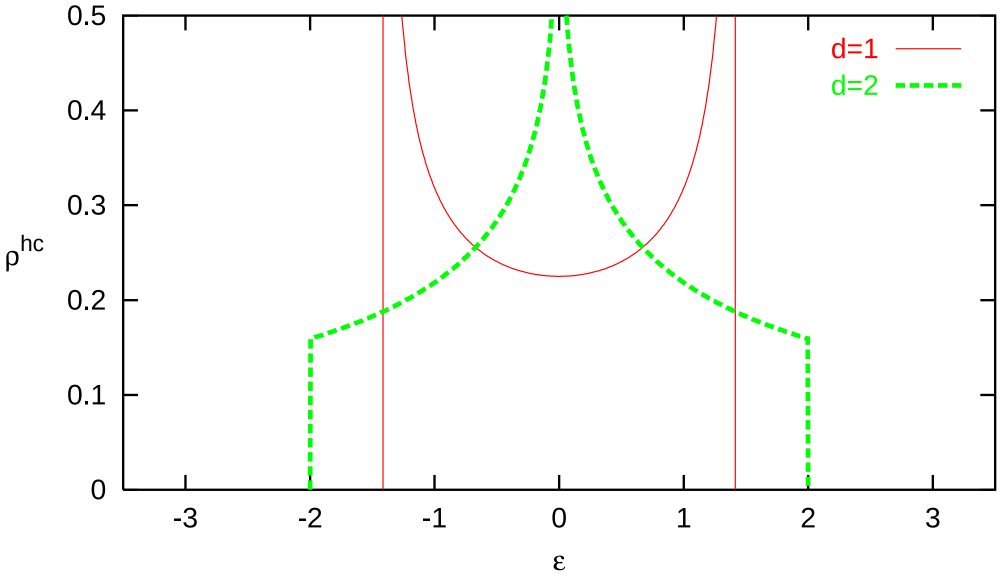

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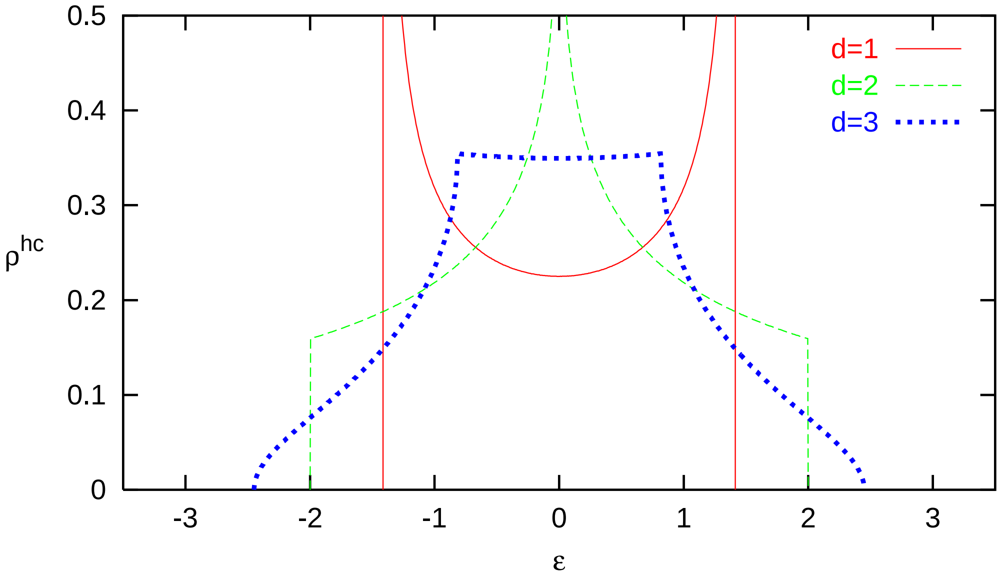

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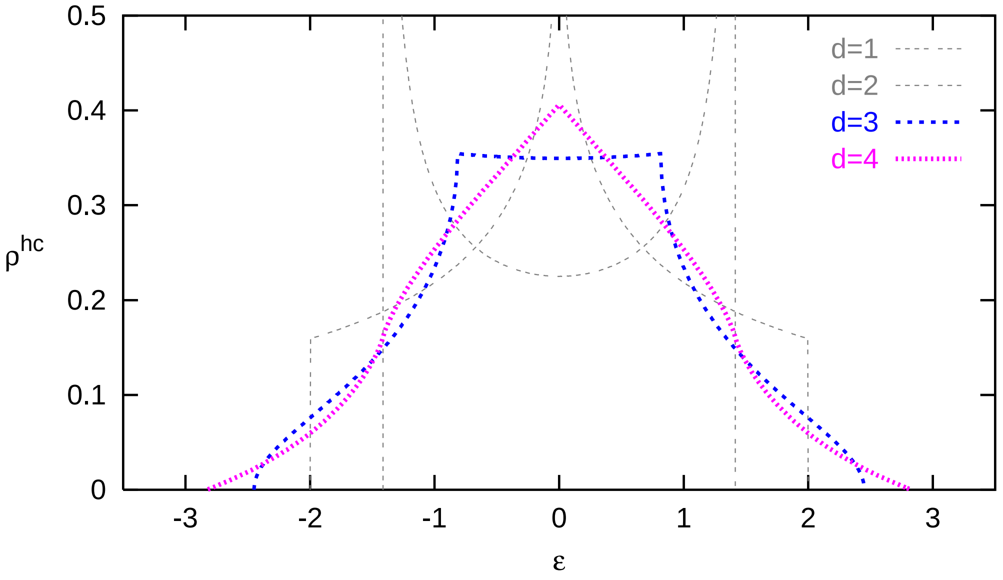

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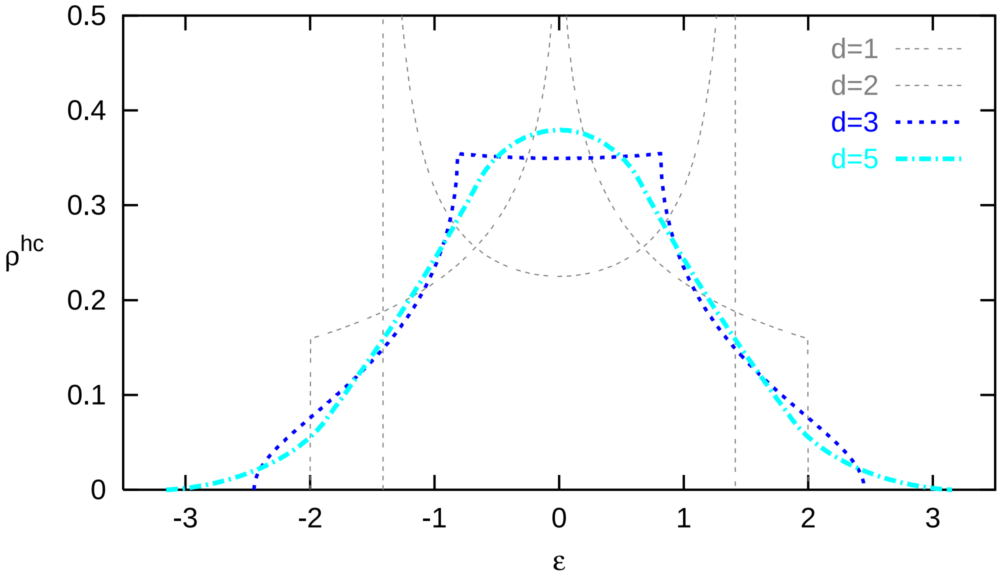

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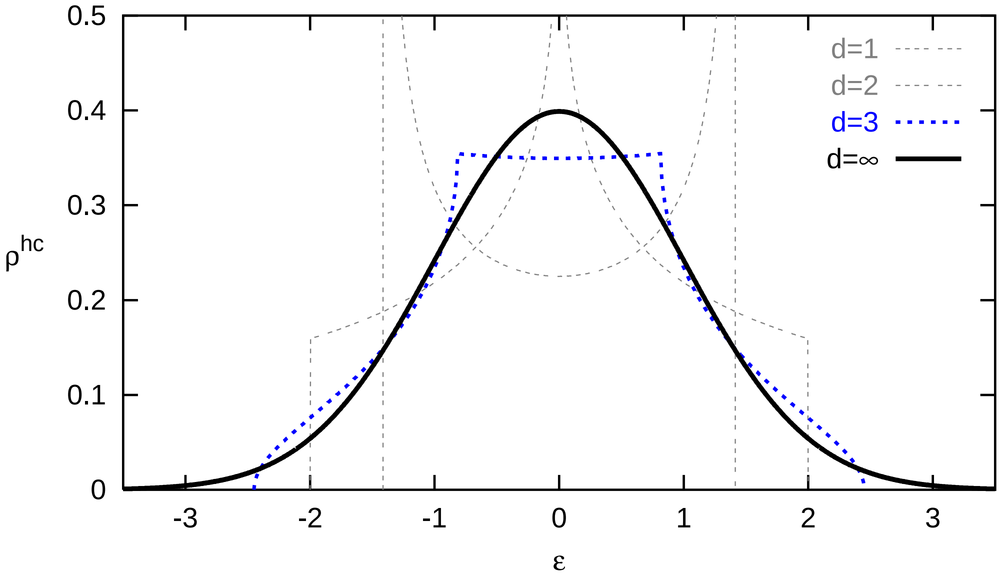

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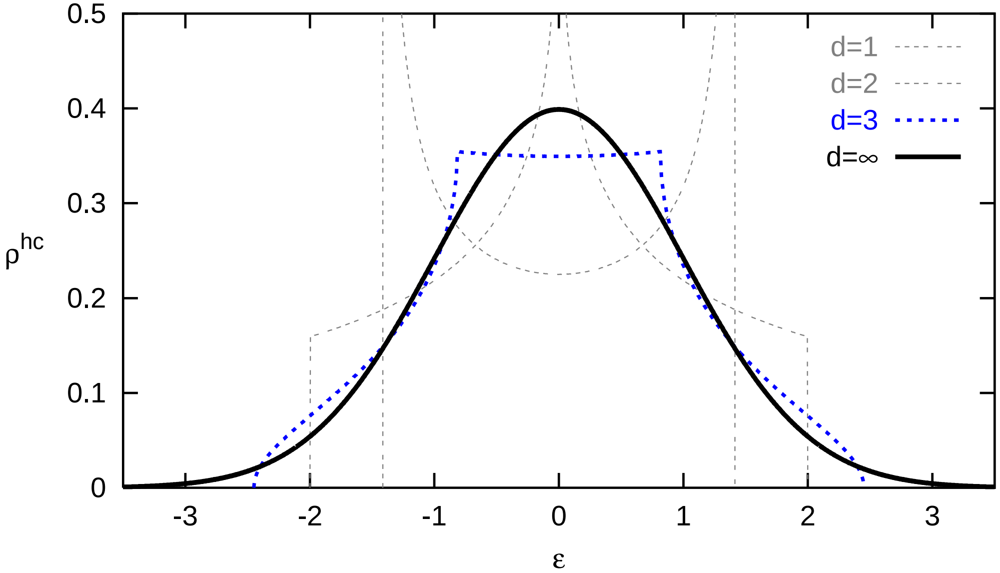

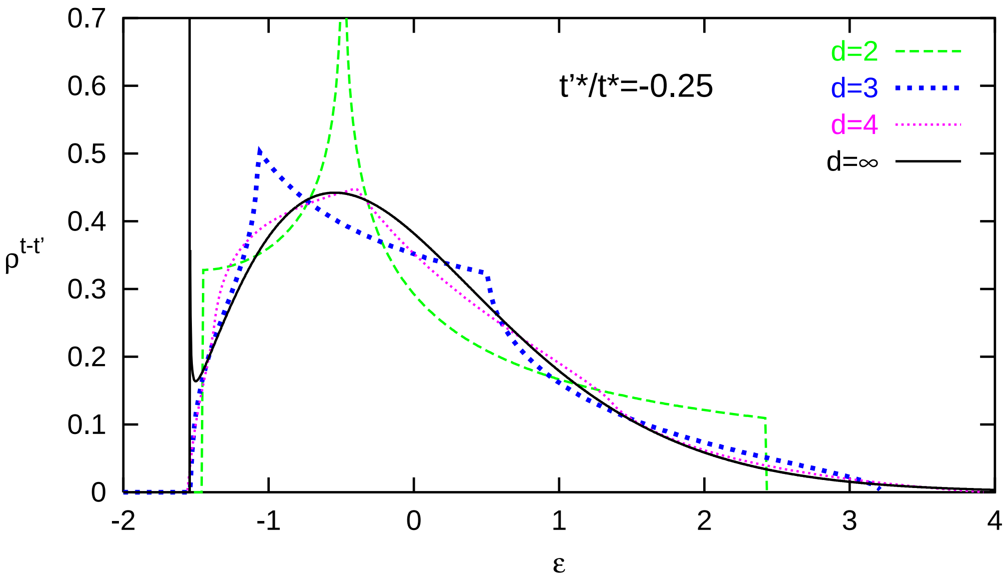

Inclusion of next-nearest neighbor hopping:

- lower band edge (for $t'^*/t^* < 0$)
- asymmetric DOS
- However: DOS still unbounded ($\Rightarrow$ no genuine band gap at large U)
- unphysical singularity at lower band edge

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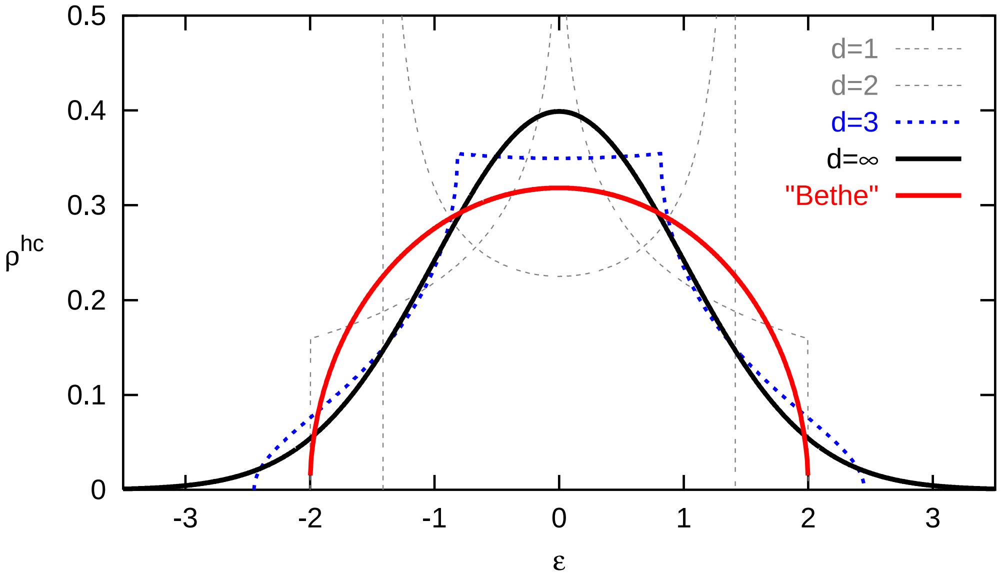

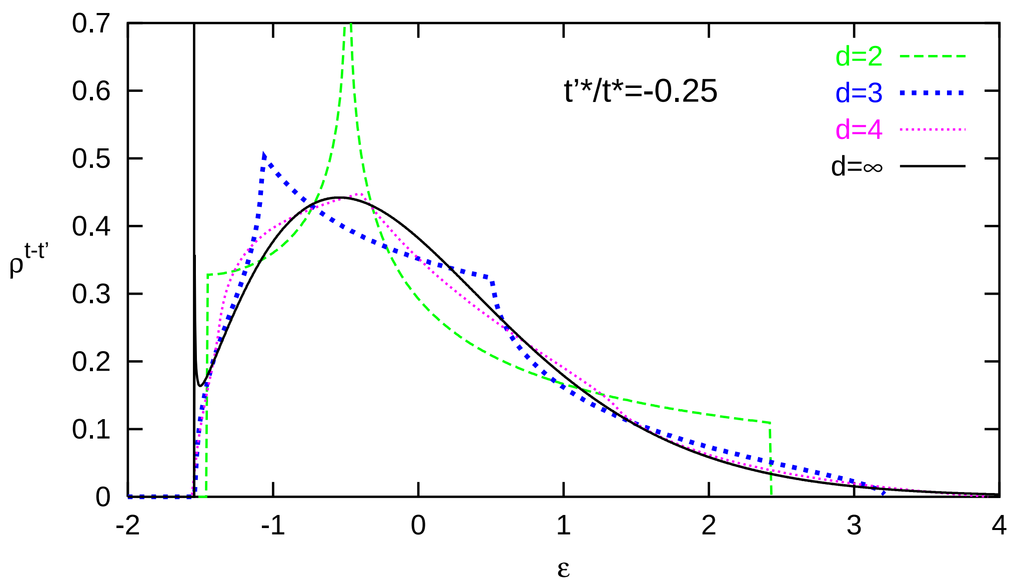

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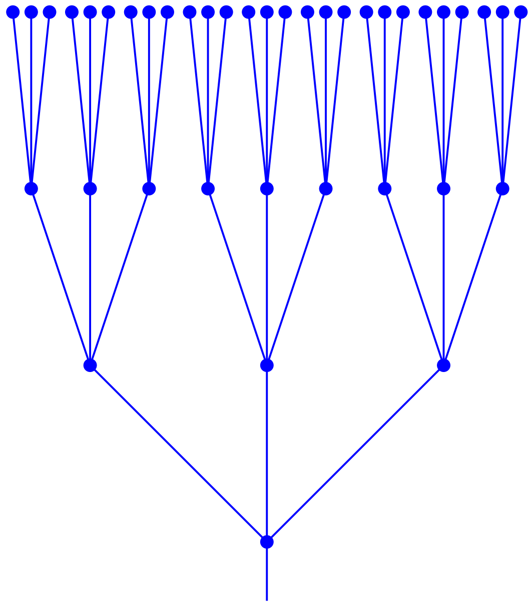
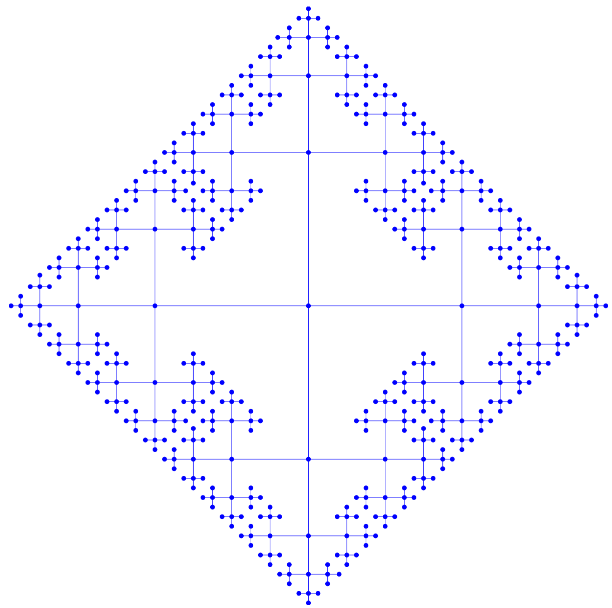
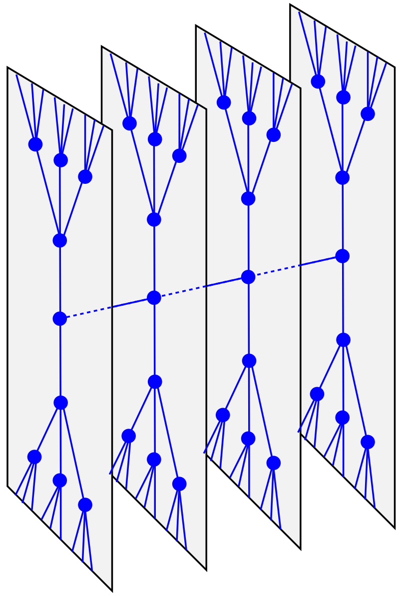
Pragmatic choice: semi-elliptic "Bethe" DOS







"Bethe lattice": defined by its topology: no loops, constant number Z of nearest neighbors

tree in the sense of graph theory

Definition suffices for computation of local properties of the homogeneous phase within DMFT

no directions, no $\boldsymbol{k}$ space: transport is a priori undefined

Semi-elliptic DOS also realized for fully disordered models [Wigner, Mattis]

DMFT Treatment of the Optical Conductivity

For continuum systems, the Kubo linear-response formalism yields:

$$\sigma_{\alpha\beta}(\omega) = \frac{V}{\hbar(\omega + i0^+)} \int_0^\infty \mathrm{d}t\, e^{i(\omega+i0^+)t} \langle [\hat{\jmath}_\alpha^\dagger(t), \hat{\jmath}_\beta(0)] \rangle + i \frac{n_0\, e^2}{m(\omega + i0^+)} \delta_{\alpha\beta}$$

In the lattice case: use Peierls construction $t_{ij} = t_{ij}^0 \, \exp\left[-i\frac{e}{c\hbar}(\boldsymbol{R}_i - \boldsymbol{R}_j)\cdot\boldsymbol{A}\right]$

derive $\hat{\boldsymbol{\jmath}}$ from $\hat{H}_0 \longrightarrow \hat{H}_0 - \frac{V}{c}\hat{\boldsymbol{\jmath}}\cdot\boldsymbol{A} + \mathcal{O}(A^2)$

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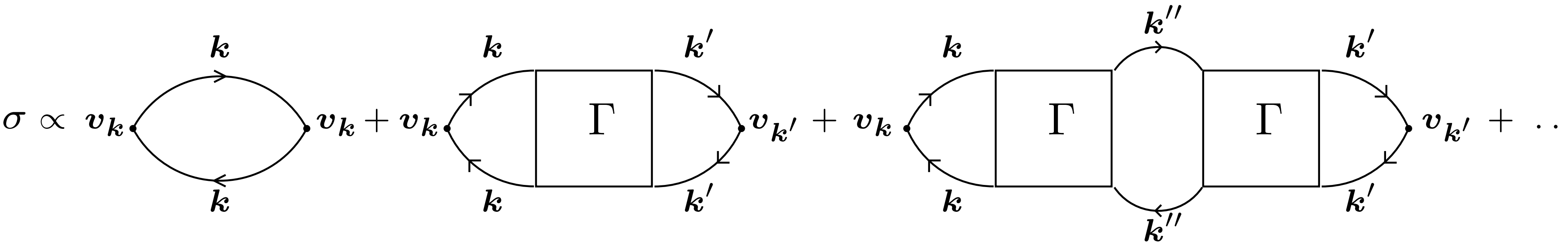
For a Bravais lattice and a single band: $\hat{\boldsymbol{\jmath}} = \frac{e}{V\hbar}\sum_{\boldsymbol{k},\sigma} \boldsymbol{v}_{\boldsymbol{k}}\, \hat{n}_{\boldsymbol{k},\sigma}$ (Fermi velocity $\boldsymbol{v}_{\boldsymbol{k}} = \frac{1}{\hbar}\nabla\epsilon_{\boldsymbol{k}}$)



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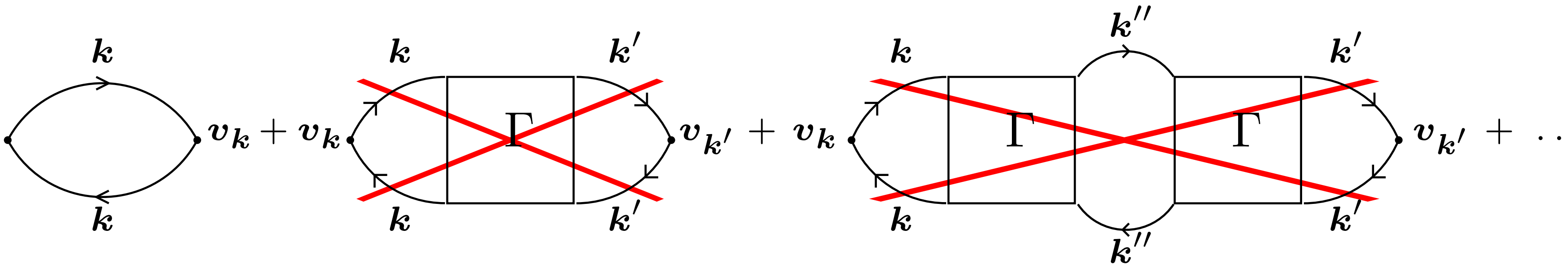
$\sigma \propto \boldsymbol{v}_{\boldsymbol{k}}$ 

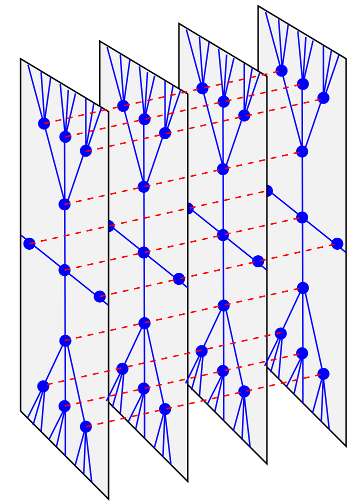
$d \to \infty$: Vertex corrections vanish [A. Khurana, Phys. Rev. Lett. **64**, 1990 (1990)]

$\boldsymbol{k}$ sum $\longrightarrow$ ϵ integral [T. Pruschke, D. L. Cox, and M. Jarrell, Phys. Rev. B **47**, 3553 (1993)]

$$\sigma_{xx}(\omega) = \sigma_0 \int_{-\infty}^{\infty} \mathrm{d}\epsilon\, \tilde{\rho}_{xx}(\epsilon) \int_{-\infty}^{\infty} \mathrm{d}\omega'\, A_\epsilon(\omega') A_\epsilon(\omega' + \omega)\, \frac{n_\mathrm{f}(\omega') - n_\mathrm{f}(\omega + \omega')}{\omega}, \quad \text{where}$$

$$\sigma_0 := \frac{2\pi e^2}{\hbar^2}\frac{N}{V}, \qquad \tilde{\rho}_{xx}(\epsilon) := \frac{1}{N}\sum_{\boldsymbol{k}} (\boldsymbol{v}_{\boldsymbol{k}})^2_x\, \delta(\epsilon - \epsilon_{\boldsymbol{k}}), \qquad A_\epsilon(\omega) := -\frac{1}{\pi}\, \mathrm{Im}\, \frac{1}{\omega - \epsilon - \Sigma(\omega)}$$

For hypercubic lattice $(\boldsymbol{v_k})_x^2$ effectively constant: $\tilde{\rho}^{\mathsf{hc}}(\epsilon) := \sum_\alpha \tilde{\rho}^{\mathsf{hc}}_{\alpha\alpha}(\epsilon) = \rho^{\mathsf{hc}}(\epsilon)$



$$\int_0^\infty \mathrm{d}\omega\, \sigma_{xx}(\omega) = -\frac{\sigma_0}{4d}\langle \hat{H}_0 \rangle$$

This generalizes to "stacked" lattices with

$$\epsilon_{\boldsymbol{k}} = \epsilon^x_{k_x} + \epsilon^\perp_{\boldsymbol{k}_\perp}\,, \qquad \sqrt{\langle(\epsilon^x_{k_x} - \langle \epsilon^x_{k_x}\rangle)^2\rangle} = \mathcal{O}(1/d)\,,$$

since then, to leading order,

$$\tilde{\rho}_{xx}(\epsilon) \;=\; \frac{1}{N}\sum_{\boldsymbol{k}} (\boldsymbol{v_k})_x^2 \delta(\epsilon - \epsilon^\perp_{\boldsymbol{k}_\perp}) \;=\; \rho(\epsilon)\,\frac{a_x}{2\pi}\int_{-\pi/a_x}^{\pi/a_x} \mathrm{d}k_x\,(\boldsymbol{v_k})_x^2 \;=\; \rho(\epsilon)\langle(\boldsymbol{v_k})_x^2\rangle\,.$$

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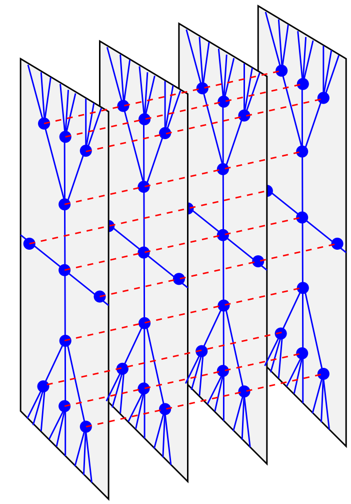

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However, the corresponding generalization of the f-sum rule is useless:

$$\int_0^\infty \mathrm{d}\omega\, \sigma_{xx}(\omega) \;=\; -\frac{\sigma_0}{4}\langle \hat{H}_{0,x}\rangle \;\neq\; -\frac{\sigma_0}{4d}\langle \hat{H}_0\rangle$$

New DMFT f-sum rule in terms of momentum distribution function $n_{\epsilon,\sigma} = \int_{-\infty}^{\infty}\mathrm{d}\omega\, n_{\mathrm{f}}(\omega)A_{\epsilon,\sigma}(\omega)$:

$$\boxed{\int_0^\infty \mathrm{d}\omega\, \sigma_{xx}(\omega) \;=\; \frac{\sigma_0}{4}\left\langle\frac{\frac{\mathrm{d}}{\mathrm{d}\epsilon}\tilde{\rho}_{xx}(\epsilon)}{\rho(\epsilon)}\right\rangle,}$$

where $\langle f(\epsilon)\rangle := \int_{-\infty}^{\infty}\mathrm{d}\epsilon\,\rho(\epsilon)\,(n_{\epsilon,\uparrow} + n_{\epsilon,\downarrow})\,f(\epsilon)$

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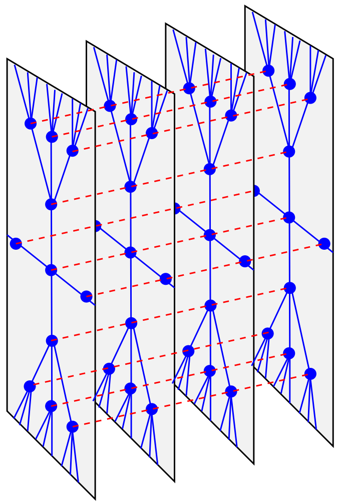


This generalizes to "stacked" lattices with

$$\epsilon_{\boldsymbol{k}} = \epsilon^x_{k_x} + \epsilon^\perp_{\boldsymbol{k}_\perp}\,, \qquad \sqrt{\langle(\epsilon^x_{k_x} - \langle\epsilon^x_{k_x}\rangle)^2\rangle} = \mathcal{O}(1/d)\,,$$

since then, to leading order,

$$\tilde{\rho}_{xx}(\epsilon) \;=\; \frac{1}{N}\sum_{\boldsymbol{k}}(\boldsymbol{v_k})_x^2\delta(\epsilon - \epsilon^\perp_{\boldsymbol{k}_\perp}) \;=\; \rho(\epsilon)\,\frac{a_x}{2\pi}\int_{-\pi/a_x}^{\pi/a_x}\mathrm{d}k_x\,(\boldsymbol{v_k})_x^2 \;=\; \rho(\epsilon)\langle(\boldsymbol{v_k})_x^2\rangle\,.$$

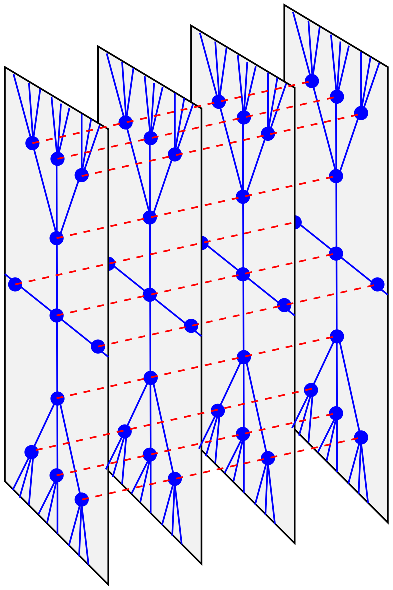
However, the corresponding generalization of the f-sum rule is useless:

$$\int_0^\infty \mathrm{d}\omega\,\sigma_{xx}(\omega) \;=\; -\frac{\sigma_0}{4}\langle\hat{H}_{0,x}\rangle \;\neq\; -\frac{\sigma_0}{4d}\langle\hat{H}_0\rangle$$

New DMFT f-sum rule in terms of momentum distribution function $n_{\epsilon,\sigma} = \int_{-\infty}^{\infty}\mathrm{d}\omega\, n_{\mathrm{f}}(\omega)A_{\epsilon,\sigma}(\omega)$:

$$\int_0^\infty \mathrm{d}\omega\,\sigma_{xx}(\omega) \;=\; \frac{\sigma_0}{4}\left\langle\frac{\frac{\mathrm{d}}{\mathrm{d}\epsilon}\tilde{\rho}_{xx}(\epsilon)}{\rho(\epsilon)}\right\rangle, \qquad \text{where } \langle f(\epsilon)\rangle := \int_{-\infty}^{\infty}\mathrm{d}\epsilon\,\rho(\epsilon)\,(n_{\epsilon,\uparrow} + n_{\epsilon,\downarrow})\,f(\epsilon)$$

Previous Approaches for the Bethe Lattice

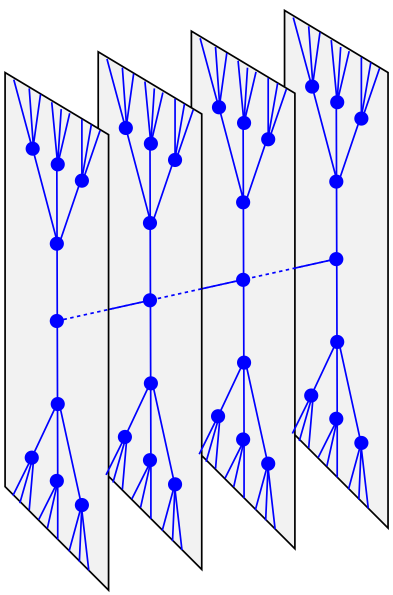


1. Periodically stacked Bethe lattice [G. S. Uhrig and R. Vlaming, J. Phys. Cond. Matter **5**, 2561 (1993)]

$$\rho(\epsilon) = \frac{1}{2\pi}\sqrt{4-\epsilon^2}, \qquad \tilde{\rho}_{xx}(\epsilon) = \frac{1}{d}\,\rho(\epsilon)$$

$$\int_0^\infty \mathrm{d}\omega\,\sigma_{xx}(\omega) \;=\; \frac{\sigma_0}{4d}\left\langle\frac{-\epsilon}{4-\epsilon^2}\right\rangle$$

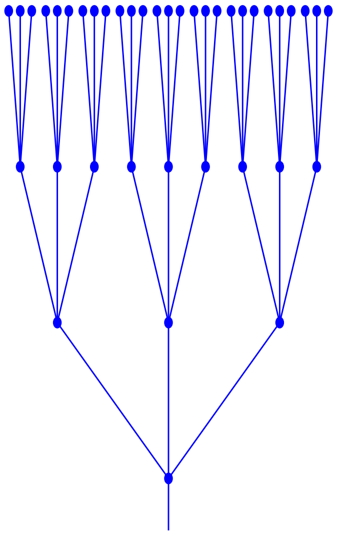
- f-sum rule contradicts [Rozenberg et al., Phys. Rev. Lett. **75**, 105 (1995)]
- transport is manifestly anisotropic



2. Single-chain layout of Bethe lattice
[M. P. H. Stumpf, Ph.D. Thesis, University of Oxford (1999)]
or full offdiagonal disorder
[V. Dobrosavljević and G. Kotliar, Phys. Rev. Lett. **71**, 3218 (1993)]

$$\sigma_{xx}(\omega) = a^2 t^2 \frac{\sigma_0}{4}\int_{-\infty}^{\infty}\mathrm{d}\omega'\,A(\omega')\,A(\omega'+\omega)\,\frac{n_{\mathrm{f}}(\omega')-n_{\mathrm{f}}(\omega+\omega')}{\omega}$$

- incoherent transport



3. Tree level picture [W. Chung and J. K. Freericks, Phys. Rev. B **57**, 11955 (1998)]

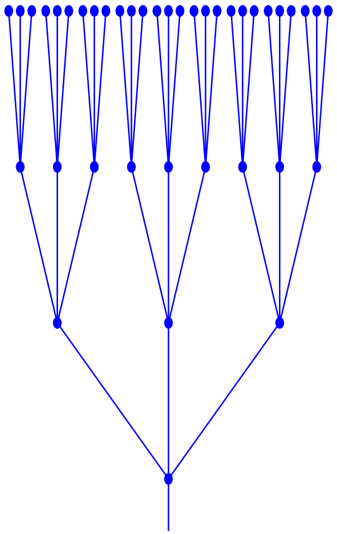
$$\text{Ansatz} \quad |\epsilon\rangle = \sum_x (\gamma_\epsilon)^x \sum_{\alpha_x} |x, \alpha_x\rangle \,, \quad \gamma_\epsilon = \frac{-\epsilon \pm \sqrt{\epsilon^2 - 4(Z-1)t^2}}{2(Z-1)t}$$

$$\Rightarrow \qquad \hat{H}_0|\epsilon\rangle = \epsilon|\epsilon\rangle, \qquad \hat{j}|\epsilon\rangle = \pm e\sqrt{4(Z-1)t^2 - \epsilon^2}|\epsilon\rangle$$

$$\overset{?}{\Longrightarrow} \quad \tilde{\rho}_{xx}(\epsilon) = \left(4{t^*}^2 - \epsilon^2\right)\rho(\epsilon), \quad \int_0^\infty \mathrm{d}\omega\, \sigma_{xx}(\omega) = 3\,\frac{\sigma_0}{4d}\,\langle -\epsilon\rangle$$

However: chosen set of states incomplete, corresponds to $\rho(\epsilon) = \dfrac{1}{\pi\sqrt{4{t^*}^2 - \epsilon^2}}$

- incomplete derivation, model effectively 1-dimensional



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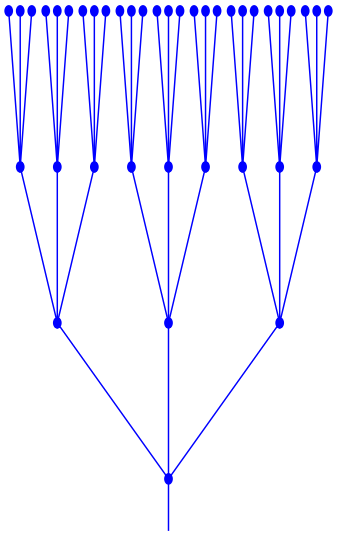

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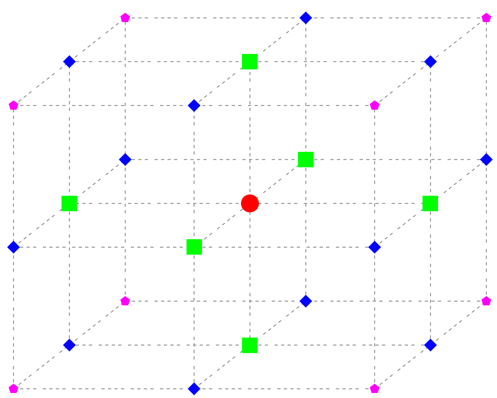

4. New: general dispersion approach

Define new microscopic model with (e.g.) semi-elliptic DOS

- regular Bravais lattice
- definition for all transport properties straightforward
- conductivity coherent in the noninteracting limit
- hypercubic symmetry, i.e., isotropic transport (for $\boldsymbol{q} \longrightarrow 0$)

General Dispersion Formalism

We rewrite the translation-invariant noninteracting Hamiltonian,

$$\hat{H}_0 = \sum_{i,\sigma} \sum_{\boldsymbol{\tau}} t_{\boldsymbol{\tau}} \; \hat{c}^{\dagger}_{\boldsymbol{R}_i+\boldsymbol{\tau},\sigma} \hat{c}_{\boldsymbol{R}_i\,\sigma} = \sum_{\boldsymbol{k},\sigma} \epsilon(\boldsymbol{k}) \hat{n}_{\boldsymbol{k}\sigma},$$

and classify contributions to the dispersion by the taxi-cab hopping distance $\|\boldsymbol{\tau}\| = \sum_{\alpha=1}^{d} |\tau_\alpha|$:

$$\epsilon(\boldsymbol{k}) = \sum_{D=1}^{\infty} \epsilon_D(\boldsymbol{k}), \qquad \epsilon_D(\boldsymbol{k}) = \sum_{\|\boldsymbol{\tau}\|=D} t_{\boldsymbol{\tau}} e^{i\boldsymbol{\tau}\cdot\boldsymbol{k}} \,.$$

For $d \to \infty$, almost all vectors $\boldsymbol{\tau}$ with $\|\boldsymbol{\tau}\| = D$ are of form $\boldsymbol{\tau} = \sum_{i=1}^{D} \boldsymbol{e}_{\alpha_i}$, $\alpha_i \neq \alpha_j$ (for $i \neq j$)

Natural choice: equivalent dimensions $\quad \Rightarrow \quad t_{\boldsymbol{\tau}} \equiv t_D = \dfrac{t_D^*}{\sqrt{N_D}}, \quad N_D = 2^D \dbinom{d}{D} \approx \dfrac{(2d)^D}{D!}$

$$\begin{aligned} \epsilon_D(\boldsymbol{k}) &= t_D \frac{2^D}{D!} \left(\frac{d}{2}\right)^{D/2} B_D(\boldsymbol{k}) \\ B_D(\boldsymbol{k}) &= \left(\frac{2}{d}\right)^{D/2} \sum_{\alpha_D \neq \alpha_{D-1} \neq \cdots \neq \alpha_1} \cos(k_{\alpha_D}) \cos(k_{\alpha_{D-1}}) \;\ldots\; \cos(k_{\alpha_1}) \end{aligned}$$

Functions $B_D(\boldsymbol{k})$ fulfill a recursion relation (to leading order)

$$
\begin{aligned}
B_{D+1}(\boldsymbol{k}) &= B_1(\boldsymbol{k})\, B_D(\boldsymbol{k}) - D\, B_{D-1}(\boldsymbol{k})\, \frac{2}{d} \sum_{\alpha=1}^{d} \cos^2(k_\alpha) + \mathcal{O}(1/d) \\
&= B_1(\boldsymbol{k})\, B_D(\boldsymbol{k}) - D\, B_{D-1}(\boldsymbol{k}) + \mathcal{O}(1/\sqrt{d})
\end{aligned}
$$

of the Hermite polynomial type. Consequently: $B_D(\boldsymbol{k}) = \mathrm{He}_D(B_1(\boldsymbol{k}))$.

With initial condition $B_1(\boldsymbol{k}) = \sqrt{\frac{2}{d}} \sum_\alpha \cos(k_\alpha) = \epsilon_{\boldsymbol{k}}^{\mathrm{hc}}$ and orthogonality relation

$\int_{-\infty}^{\infty} \mathrm{d}x\, \mathrm{He}_n(x)\, \mathrm{He}_m(x)\, \frac{e^{-x^2/2}}{\sqrt{2\pi}} = n!\, \delta_{mn}$:

$$
\epsilon(\boldsymbol{k}) = \sum_{D=1}^{\infty} \frac{t_D^*}{\sqrt{D!}}\, \mathrm{He}_D(\epsilon_{\boldsymbol{k}}^{\mathrm{hc}}) =: \mathcal{F}(\epsilon_{\boldsymbol{k}}^{\mathrm{hc}})
$$

$$
t_D^* = \frac{1}{\sqrt{2\pi D!}} \int_{-\infty}^{\infty} \mathrm{d}\epsilon\, \mathcal{F}(\epsilon)\, \mathrm{He}_D(\epsilon)\, e^{-\epsilon^2/2}
$$

so far: completely general (for equivalent dimensions and usual DMFT scaling)

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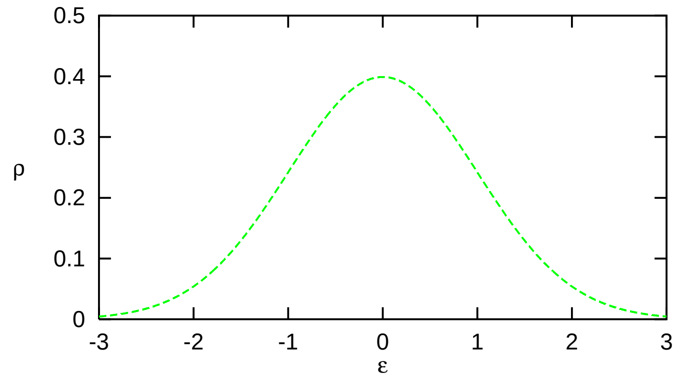
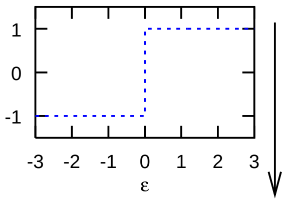
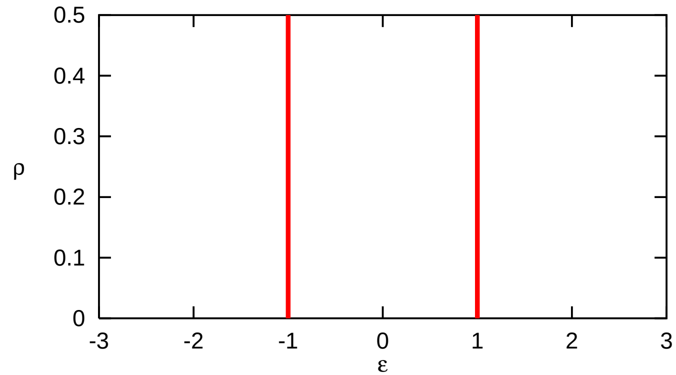
Choice of monotonic transformation function $\mathcal{F}(x)$ implies $\rho(\epsilon) = \frac{1}{\mathcal{F}'(\mathcal{F}^{-1}(\epsilon))}\, \rho^{\mathrm{hc}}(\mathcal{F}^{-1}(\epsilon))$ and

$$\mathcal{F}^{-1}(\epsilon) = \sqrt{2}\, \mathrm{erf}^{-1}\left(2 \int_{-\infty}^{\epsilon} \mathrm{d}\epsilon'\, \rho(\epsilon') - 1\right)$$





$\mathcal{F}(x) = 2\Theta(x) - 1$



Example 1: Flat-band System

DOS $\rho(\epsilon) = \frac{1}{2}\big(\delta(\epsilon - 1) + \delta(\epsilon + 1)\big)$.

Hopping matrix elements (trivially, $t^*_{2n} = 0$):

$$t^*_{2n+1} = (-1)^n \sqrt{\frac{2}{\pi}} \frac{(2n-1)!!}{\sqrt{(2n+1)!}} \overset{n\to\infty}{\longrightarrow} (-1)^n (\pi n)^{-3/4}$$

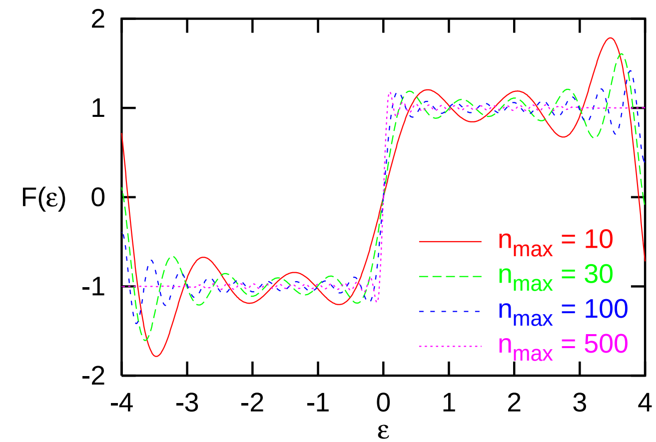
asymptotic exponent $-\frac{3}{4}$

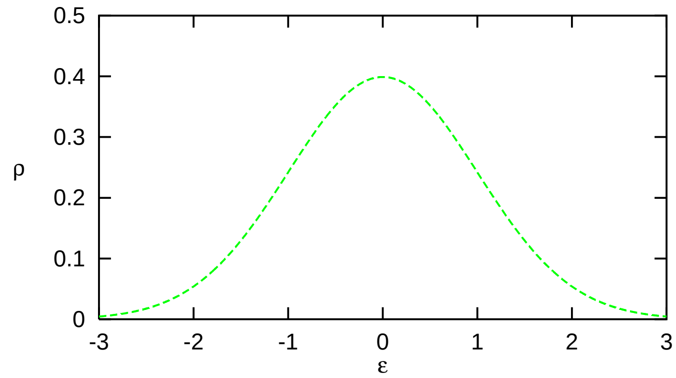
below threshold value $-\frac{1}{2}$

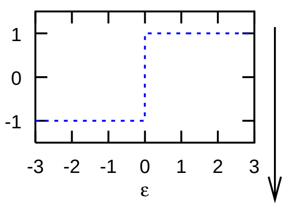
required for finite variance

$\langle \epsilon^2(\boldsymbol{k})\rangle = \sum_D {t^*_D}^2$

slow convergence of $\mathcal{F}$







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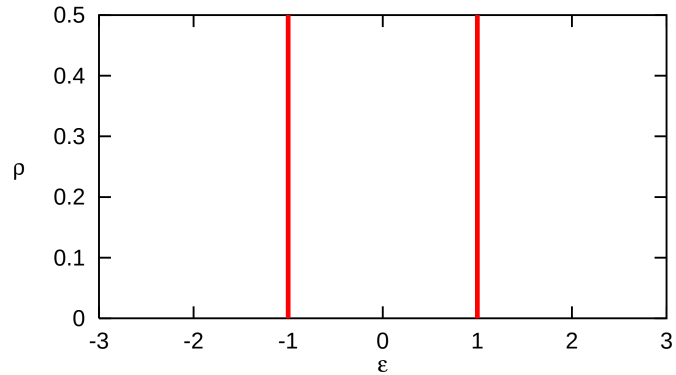

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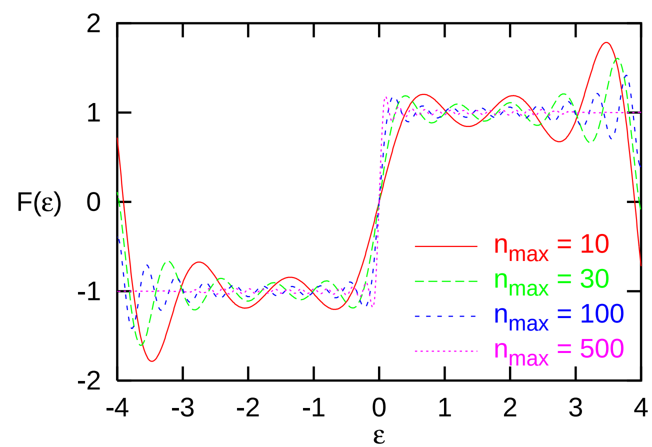
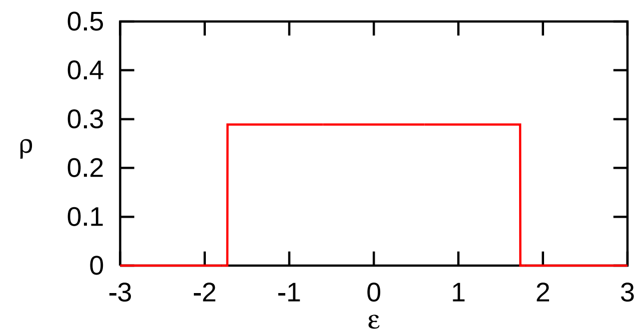


Example 2: constant DOS

rectangular model DOS: $\rho(\epsilon) = \frac{1}{2\sqrt{3}}\Theta(\sqrt{3} - \epsilon)$

decay of t^*_D is already exponential

$$t^*_{2n+1} = (-1)^n \sqrt{3}\pi \frac{(2n)!}{2^{2n} n! \sqrt{(2n+1)!}} \sim 2^{-n} n^{-3/4}$$

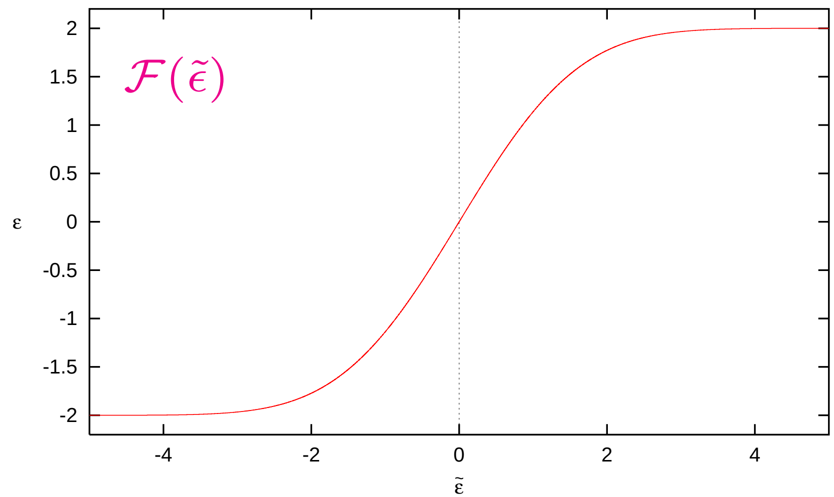


Redefinition of the Bethe Lattice

For semi-elliptic DOS, $\rho(\epsilon) = \frac{1}{2\pi}\sqrt{4-\epsilon^2}$:

$$\mathcal{F}^{-1}(\epsilon) = \frac{\sqrt{2}}{\pi}\mathrm{erf}^{-1}\left[\epsilon\sqrt{1-(\epsilon/2)^2}+2\arcsin(\epsilon/2)\right]$$

numerical inversion $\rightsquigarrow$ $\mathcal{F}(\tilde{\epsilon})$



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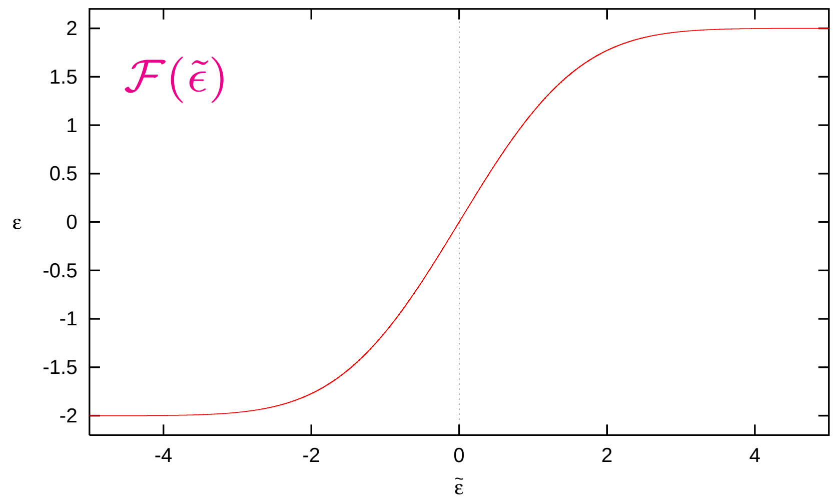

D	t_D^*	$\sum_{n=1}^{D} {t_n^*}^2$
1	0.98731	0.974773
3	-0.15353	0.998345
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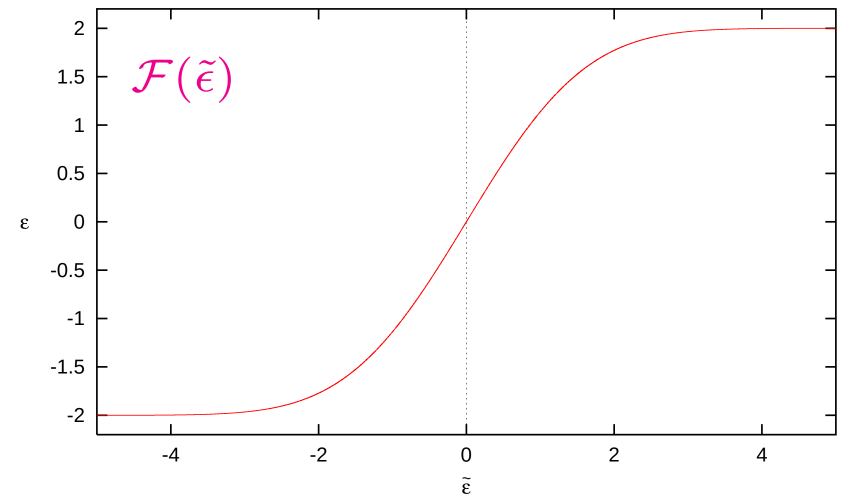
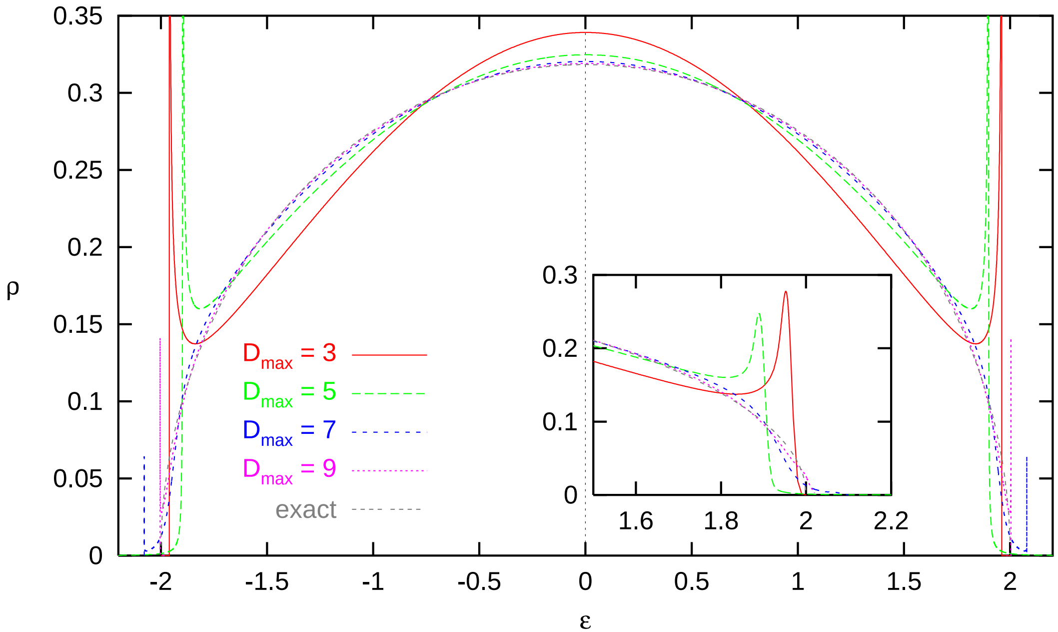
numerical integration $\rightsquigarrow t_D^*$

fast convergence with maximal hopping distance $D_{\max}$





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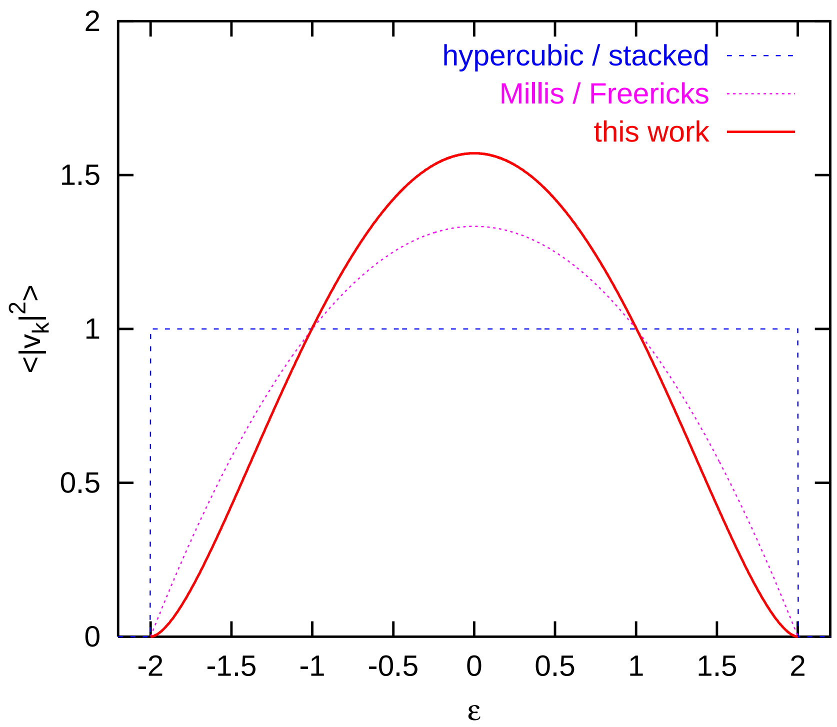
Chain rule yields Fermi velocity in general dispersion formalism: $\boldsymbol{v}_{\boldsymbol{k}} = \mathcal{F}'(\mathcal{F}^{-1}(\epsilon))\boldsymbol{v}_{\boldsymbol{k}}^{\mathsf{hc}}$.

Specifically, for Bethe semi-elliptic DOS:

$$\langle|\boldsymbol{v}_{\boldsymbol{k}}|^2\rangle(\epsilon) := \frac{\tilde{\rho}(\epsilon)}{\rho(\epsilon)} = \frac{\pi}{2(1-\epsilon^2/4)} \exp\left[-2\left(\mathrm{erf}^{-1}\left(\frac{\epsilon\sqrt{1-\epsilon^2/4}+2\arcsin(\epsilon/2)}{\pi}\right)\right)^2\right].$$



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- effect even stronger than found/assumed by Freericks and Millis
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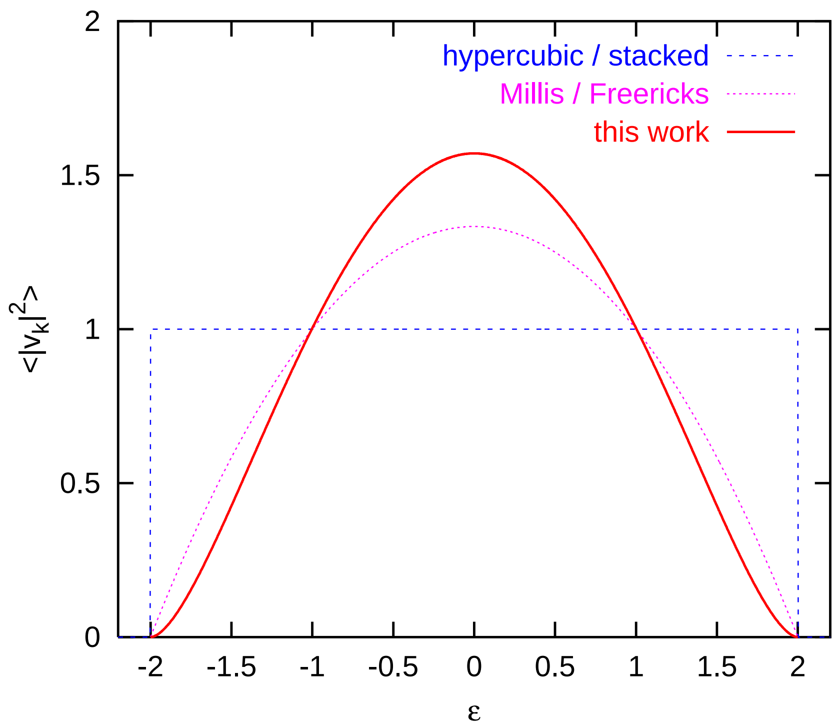

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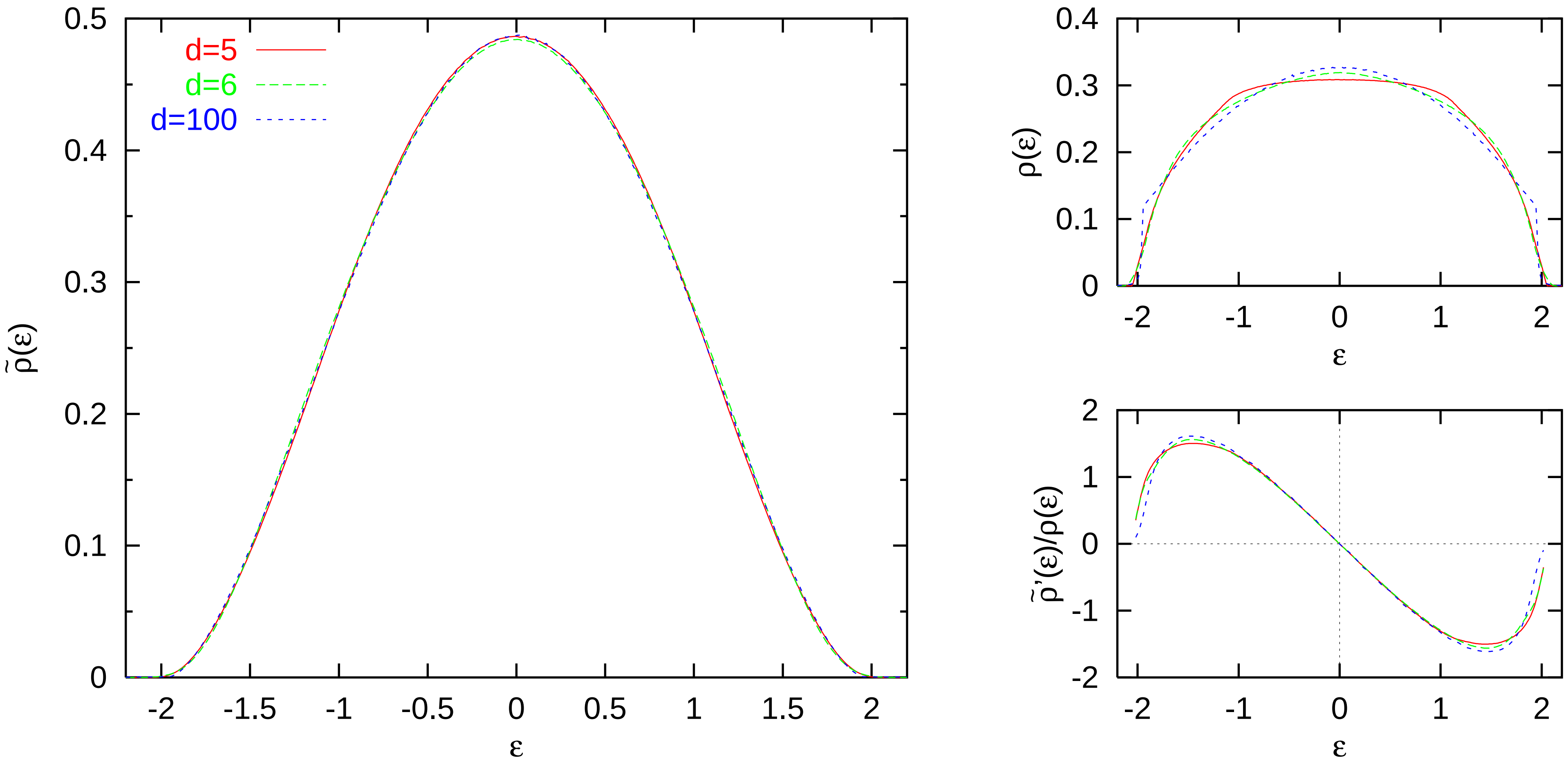
f-sum rule: $$\int_0^\infty d\omega\, \sigma_{xx}(\omega) = \frac{\sigma_0}{4d}\left\langle\frac{\tilde{\rho}'(\epsilon)}{\rho(\epsilon)}\right\rangle = \frac{\sigma_0}{4d}\left\langle\left[\mathcal{F}''(\mathcal{F}^{-1}(\epsilon)) - \mathcal{F}^{-1}(\epsilon)\mathcal{F}'(\mathcal{F}^{-1}(\epsilon))\right]\right\rangle$$

Test for robustness: finite hopping range and finite dimensionality



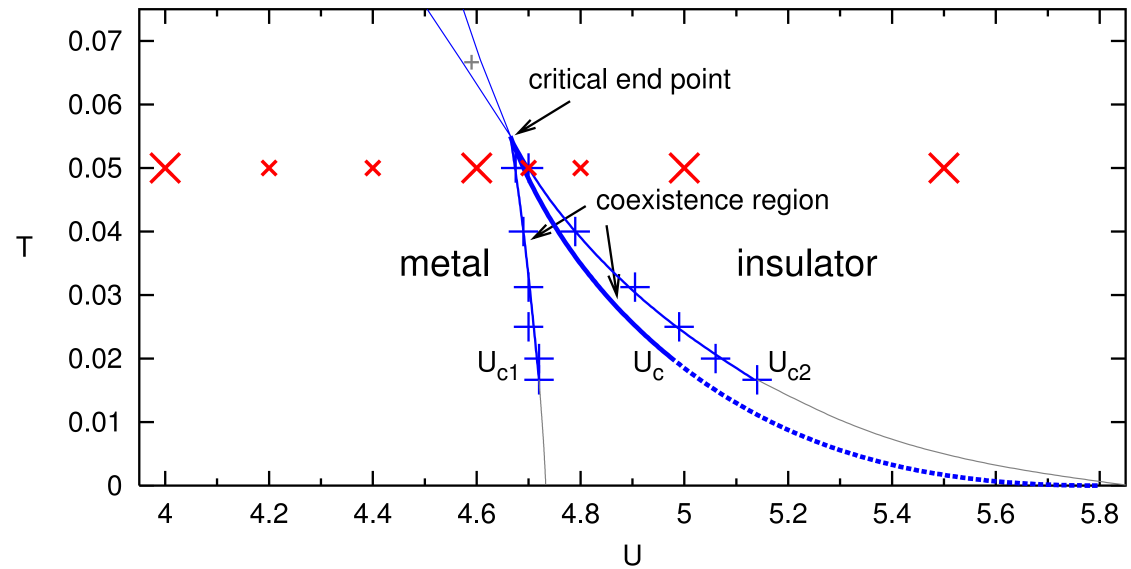
Restriction to 5^{th} nearest neighbor hopping leads to a slight suppression of $\tilde{\rho}(\epsilon)$

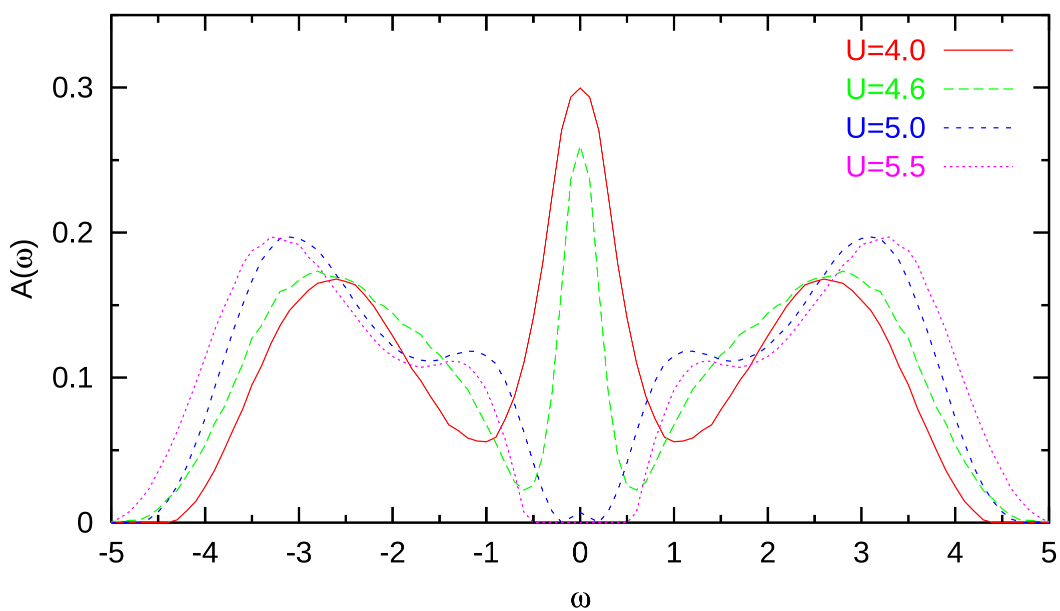
Dimensional dependence negligible, even smaller than for DOS $\rho(\epsilon)$

Numerical Results for $\sigma(\omega)$ and f-sum

Hubbard model: $n = 1$, Bethe DOS

Metal-insulator transition region for $4.0 \leq U \leq 5.5$ and $T = 0.05$, just below $T^* \approx 0.055$

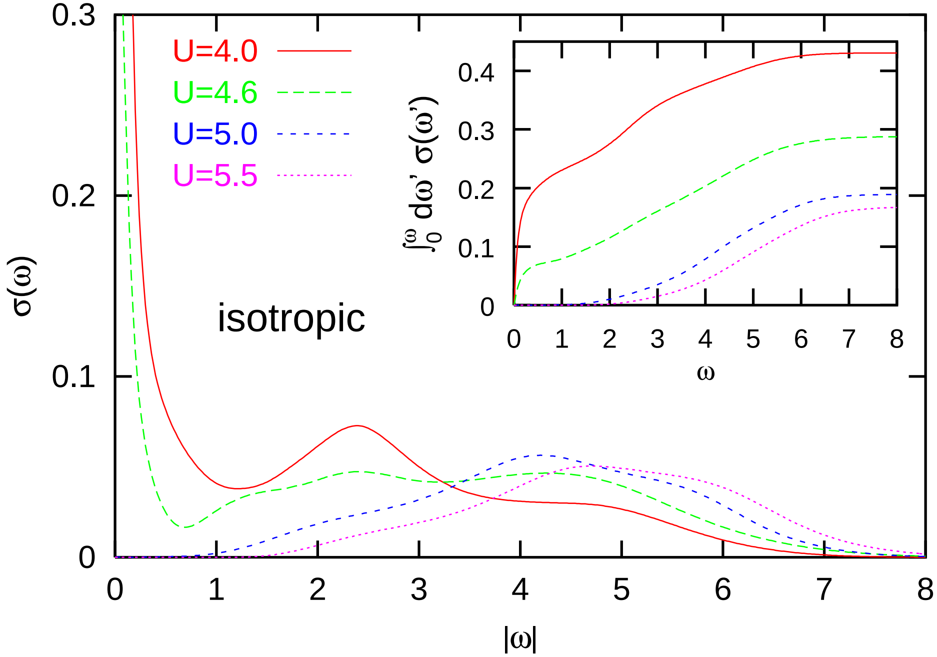




QMC with time discretization $\Delta\tau = 0.1$

MEM using flat default model

- good Luttinger pinning for $U \lesssim 4.4$
- quasiparticle peak disappears at the transition ($U \approx 4.7$)
- gap opens for $U \gtrsim 4.8$



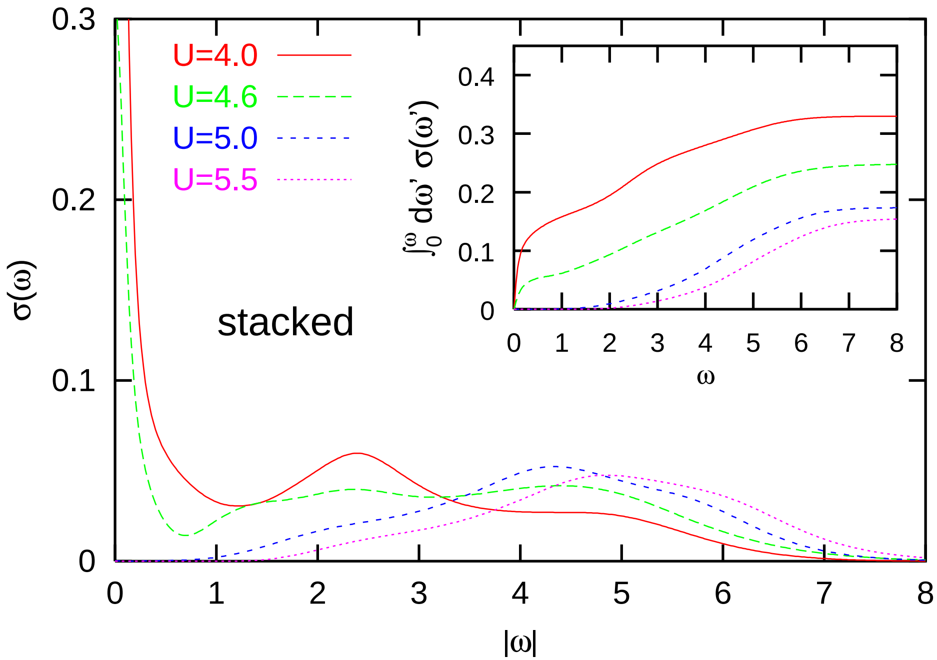
in metallic phase ($U = 4.0$, $U = 4.6$):

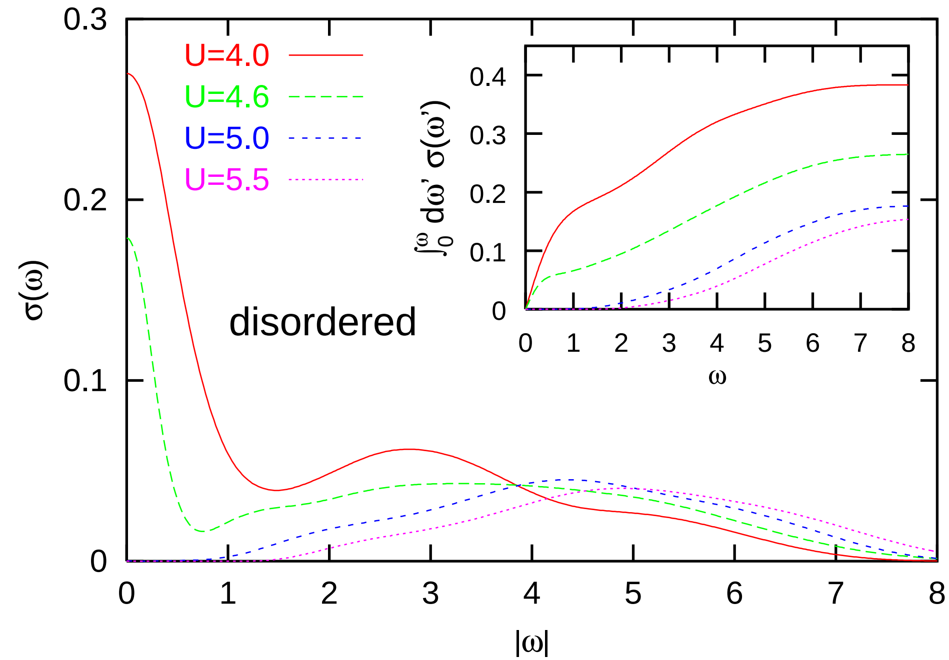
- low-frequency Drude peak
- mid-infrared peak at $\omega \approx U/2$

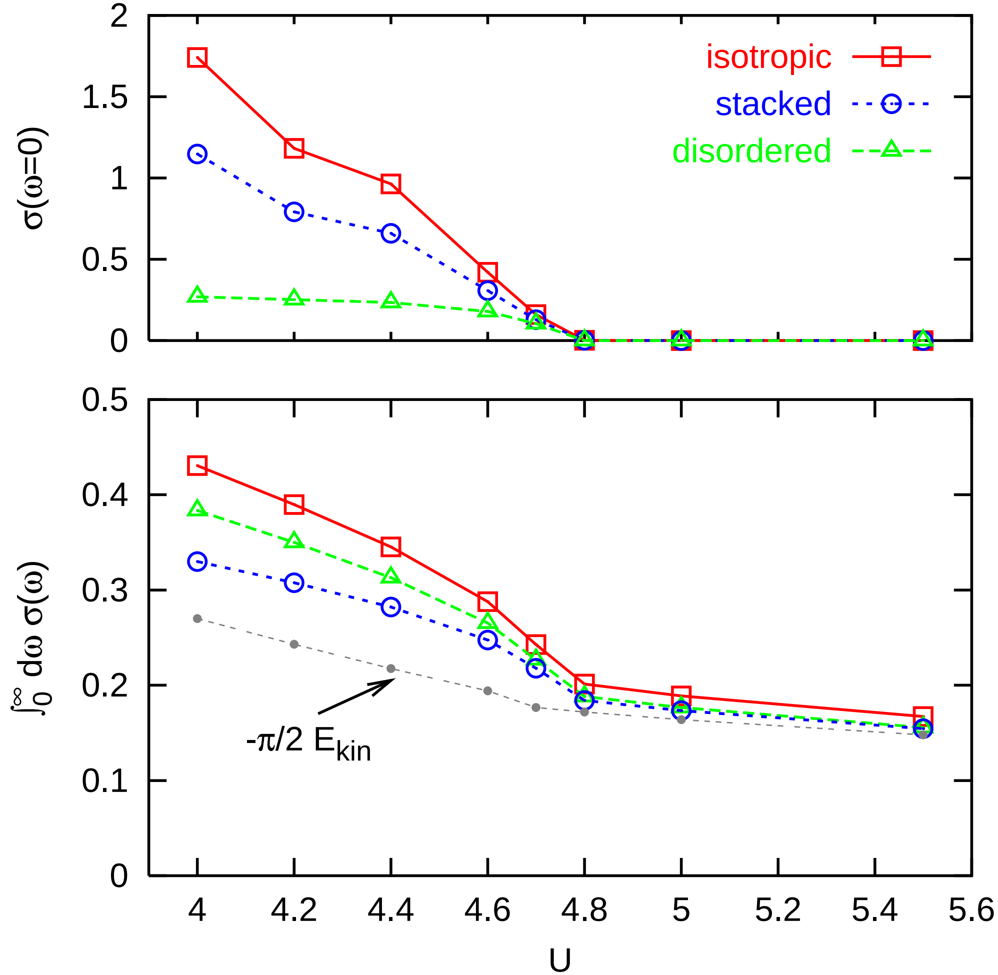
incoherent peaks at $\omega \approx U$ remain for large U

largest contributions at small ω for isotropic def

no Drude peaks for incoherent definitions







$\sigma(\omega)$ and f-sum largest for isotropic clean case

enhancement strongest in coherent (metallic) phase due to enhanced $\tilde{\rho}(\epsilon)$ at $\epsilon \approx 0$ by factor $\pi/2 \approx 1.57$

in incoherent limit enhancement by

$$\int_{-\infty}^{\infty} d\epsilon\, \tilde{\rho}(\epsilon) = \sum_{D=1}^{\infty} D\, {t_D^*}^2 \approx 1.054$$

much smaller σ_{dc} in disordered / single-chain case, intermediate f-sum

In all cases, proportionality of the f-sum to the kinetic energy clearly violated (at finite U and T)

Conclusion

previously: discussion of transport in high dimensions restricted to

- systems with unbounded density of states
- strongly anisotropic "stacked" models
- incoherent systems with full hopping disorder

new general method for constructing regular lattice models with hypercubic symmetry and arbitrary DOS in large dimensions

- first regular and clean lattice (nonsingular $\mathbf{v}_\mathbf{k}$) with sharp (3d like) band edges in $d \to \infty$ see also: [M. Kollar, Int. J. Mod. Phys. B, **16**, 3491 (2002)]
- first definition of isotropic and coherent optical conductivity $\sigma(\omega)$ in high dimensions consistent with Bethe semi-elliptic DOS
- small impact of truncation of hopping range and application in finite dimensions

new DMFT f-sum rule

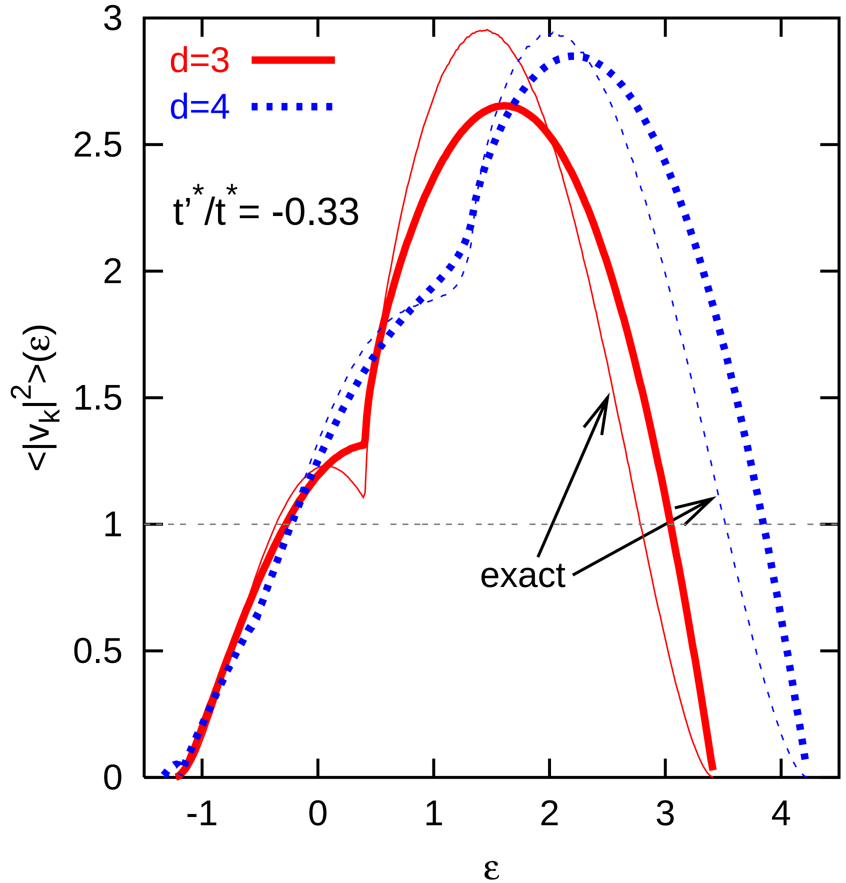
numerical results for $\sigma(\omega)$ based on high-precision QMC/MEM spectra

general dispersion formalism useful as heuristic scheme in finite dimensions when locality of Σ and Γ are used as approximations

not discussed: vertex corrections and reduced umklapp scattering in finite dimensions, multiple bands

General dispersion formalism as heuristic scheme

Test: $t - t'$ model



Application for t_{2g} bands of $La_{1\text{-}x}Sr_xTiO_3$ based on LDA data