

Optical Conductivity of Strongly Correlated Electron Systems in High Dimensions

N. Blümer

Universität Mainz

Outline

1. Introduction
2. DMFT Treatment of the Optical Conductivity
3. Previous Approaches for the Bethe Lattice
4. General Dispersion Formalism
5. Numerical QMC/MEM Results for $\sigma(\omega)$ and f -sum
6. Conclusion

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Introduction

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

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

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

Homogeneous system, long-wavelength limit $\mathbf{q} \rightarrow 0$:

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

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

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

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Connection with Reflectivity and Experiment

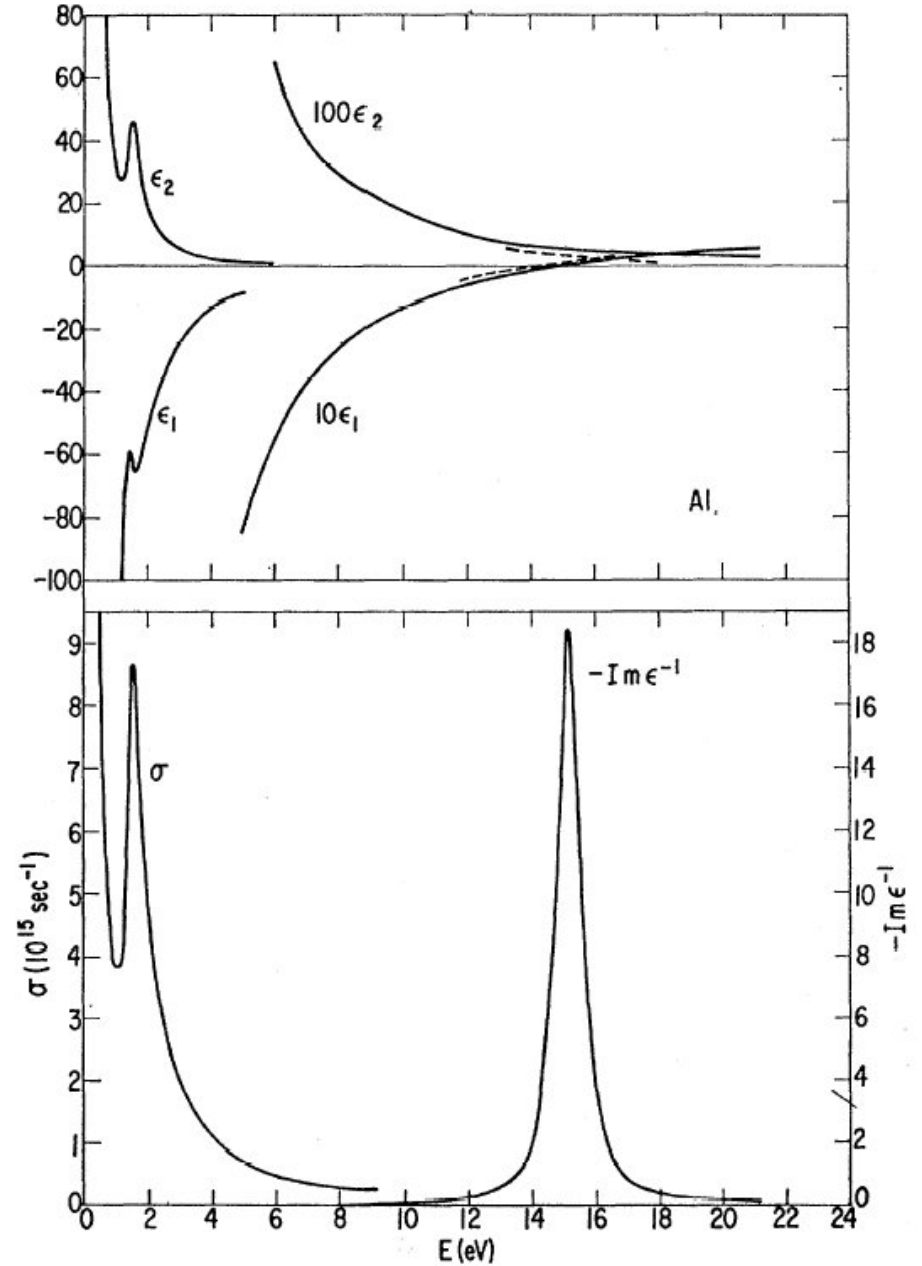
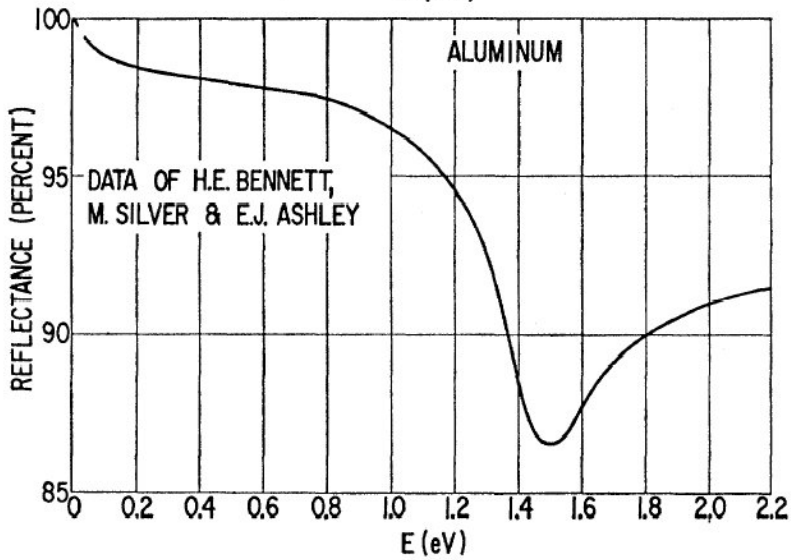
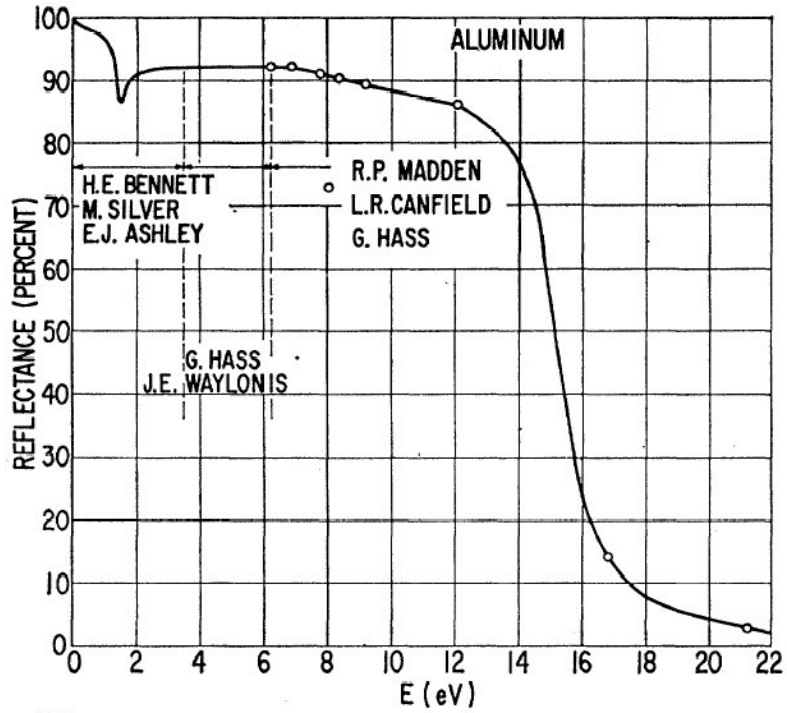
Dielectric function $\epsilon(\omega) = 1 + \frac{4\pi i}{\omega} \sigma(\omega)$ and $\kappa(\omega) \equiv \sqrt{\epsilon(\omega)}$ also analytic

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 energy spectrum:

$$\epsilon(\omega) \xrightarrow{\omega \rightarrow \infty} 1 - \frac{\omega_p^2}{\omega^2}$$

$$\frac{2}{\pi} \int_0^\infty d\omega \omega \operatorname{Im} \epsilon(\omega) = \omega_p^2$$

$$\Rightarrow \left\{ \begin{array}{l} \int_0^\infty d\omega \operatorname{Re} \sigma(\omega) = \frac{\omega_p^2}{8} \\ \int_0^\infty d\omega \omega \operatorname{Im} \kappa(\omega) = \frac{\pi}{4} \omega_p^2 \\ \int_0^\infty d\omega \omega \operatorname{Im} \frac{-1}{\epsilon(\omega)} = \frac{\pi}{2} \omega_p^2 \end{array} \right. \quad \begin{array}{l} \text{Optical} \\ f\text{-sum rule} \end{array}$$

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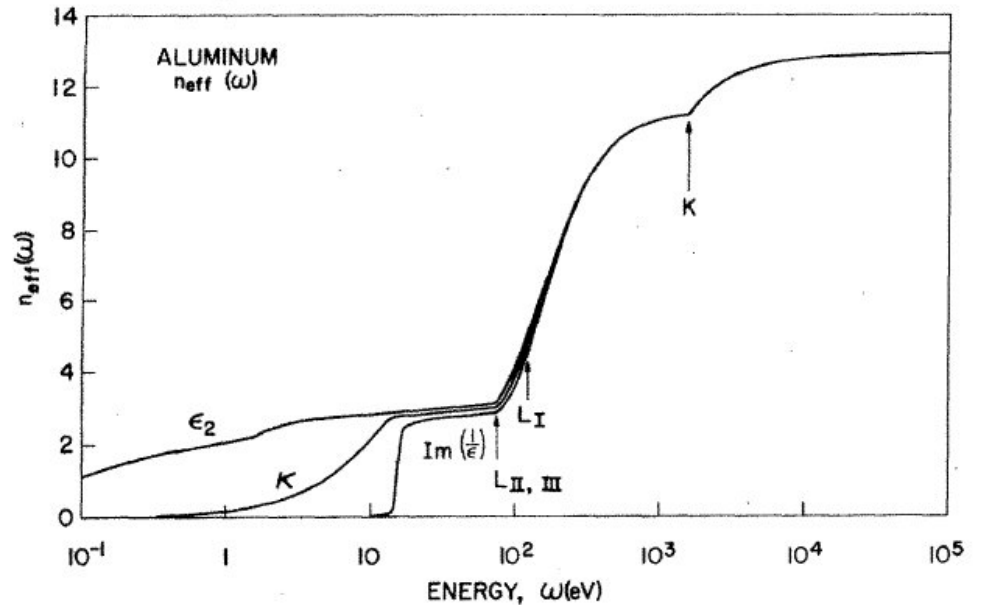
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Full **universal** f -sum rule: $\omega_p^2 = \frac{4\pi n e^2}{m}$

frequency cutoff $\omega_c \longrightarrow$ partial sum rules

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

non-universal!



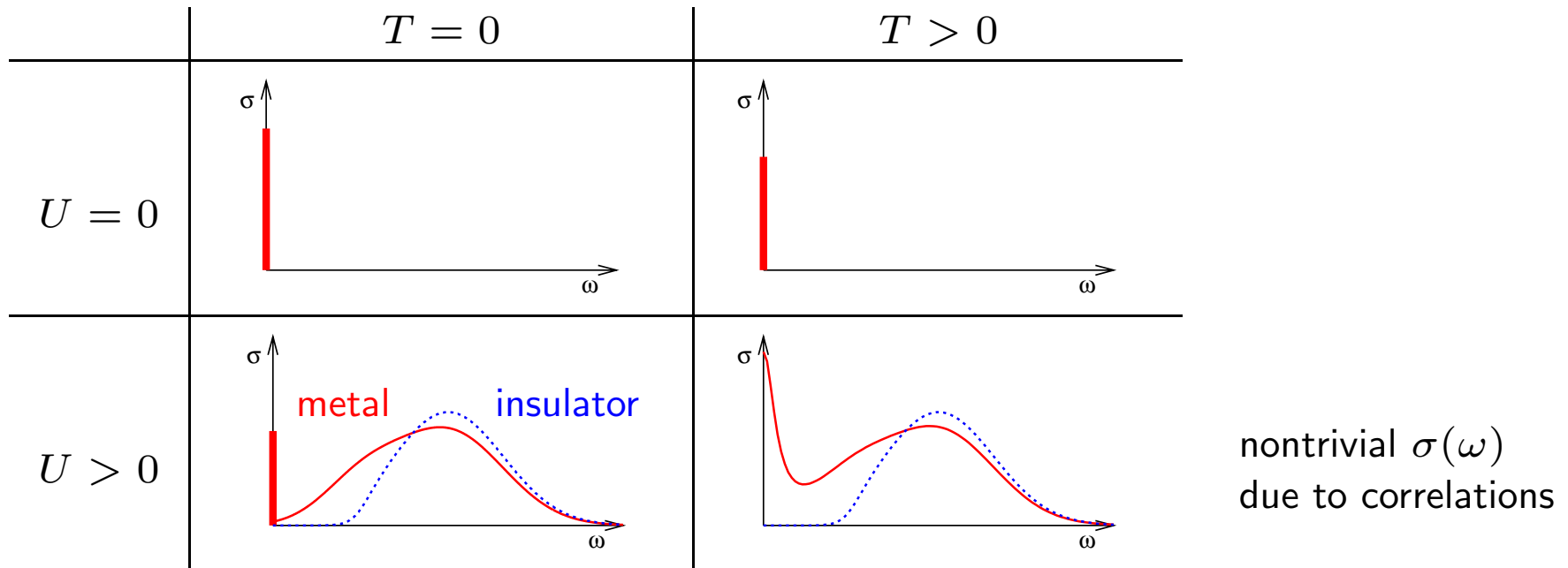
[D. Y. Smith and E. Shiles, Phys. Rev. B **17**, 4689 (1978)]

Lattice Model

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

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

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



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

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

Density of States (DOS) in High Dimensions

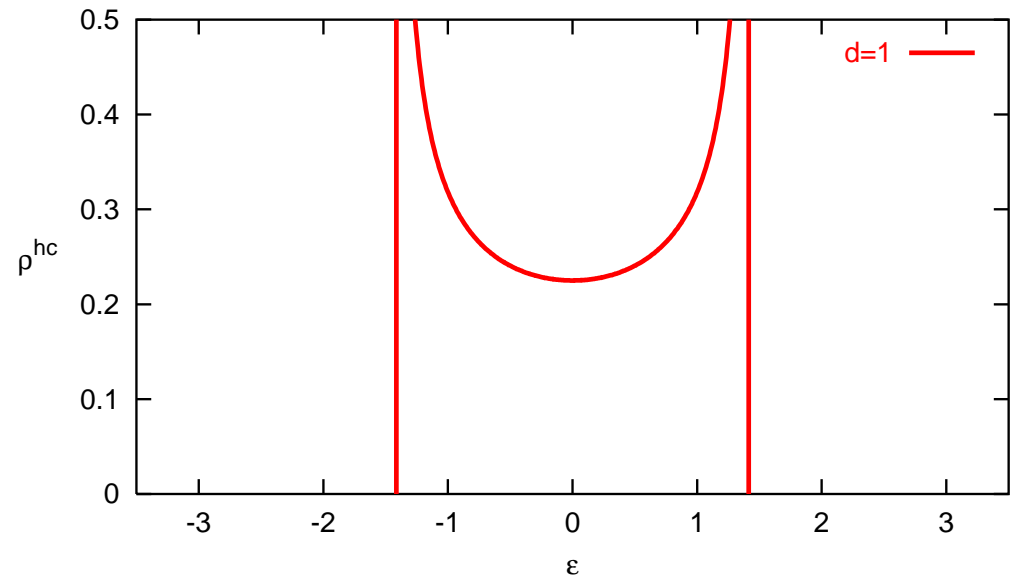
For uniform nearest neighbor (NN) hopping on a hypercubic (hc) lattice:

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

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

for $d \rightarrow \infty$: 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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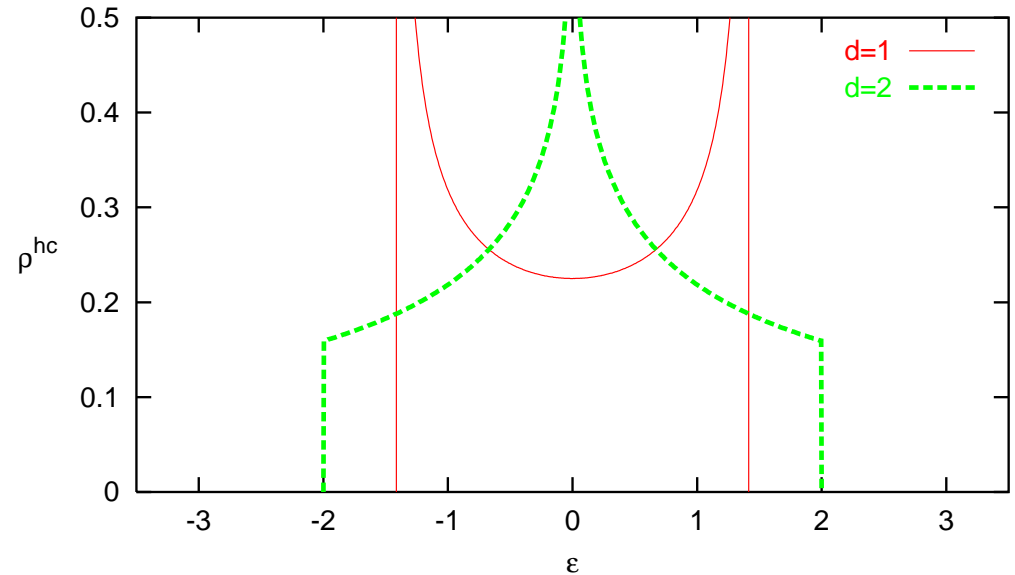
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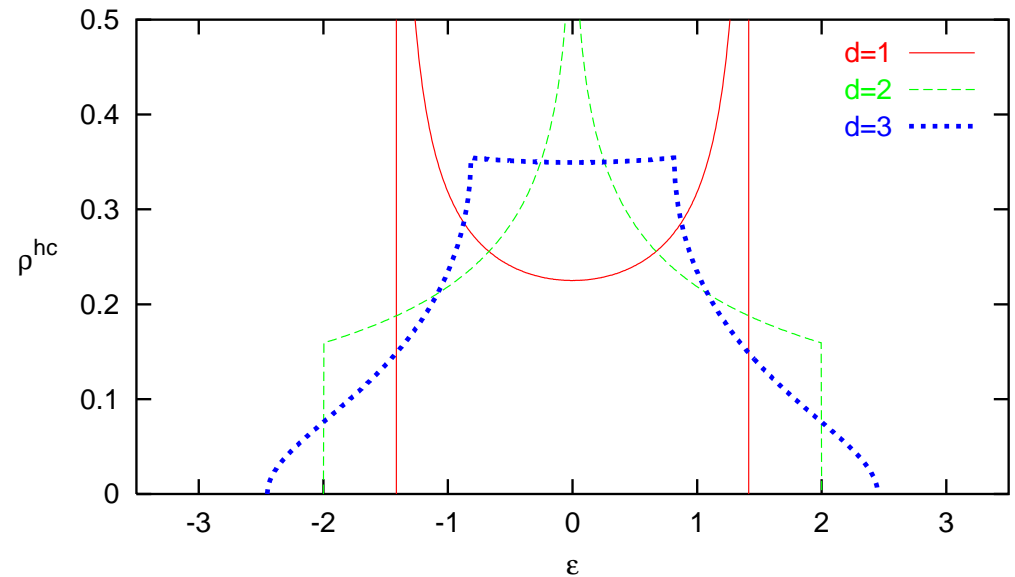
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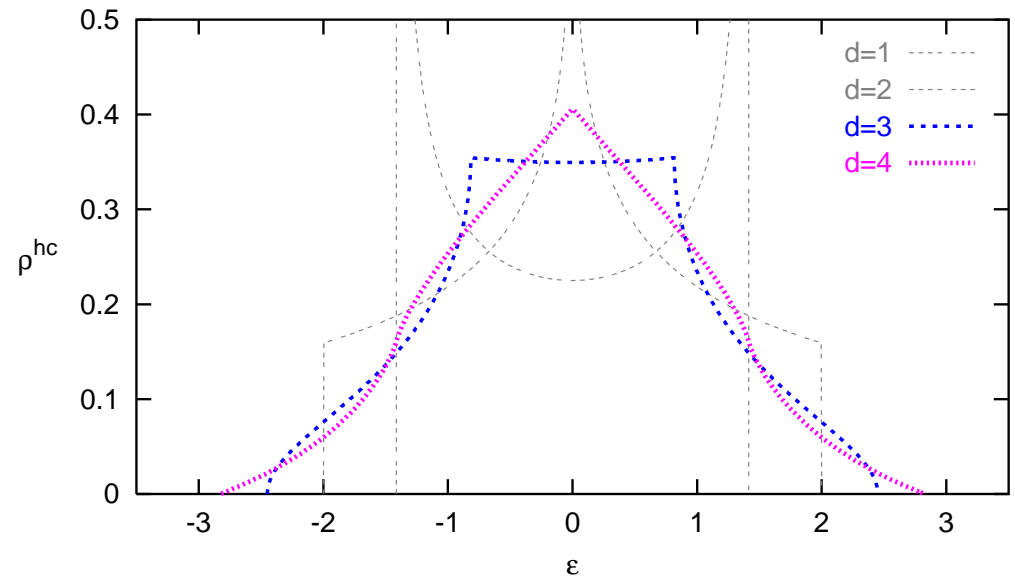
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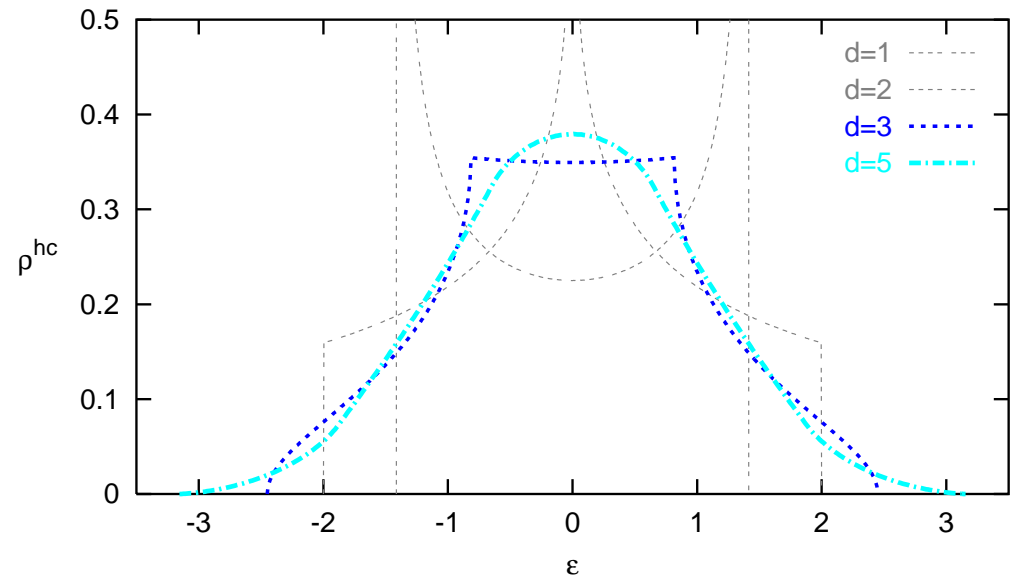
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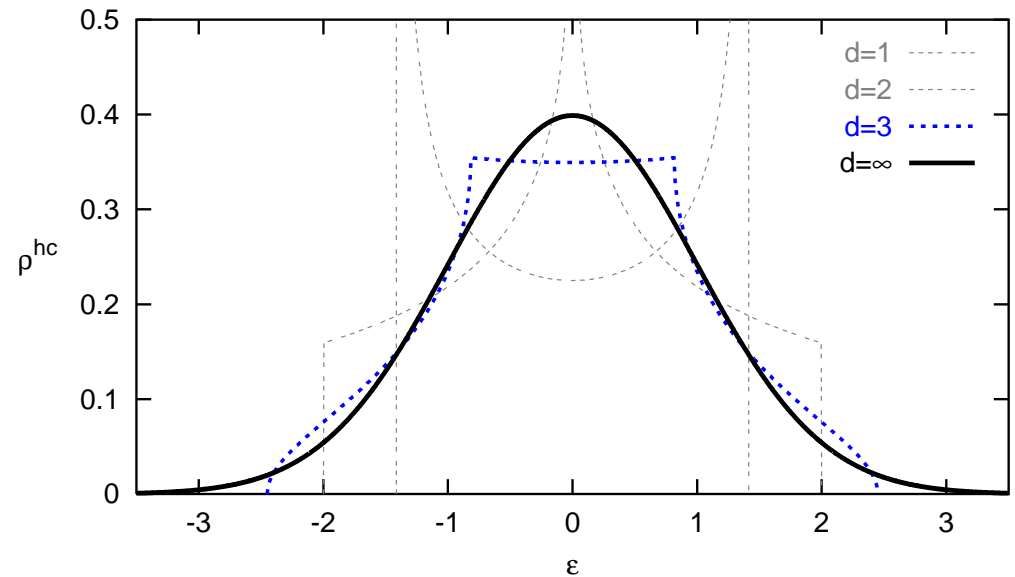
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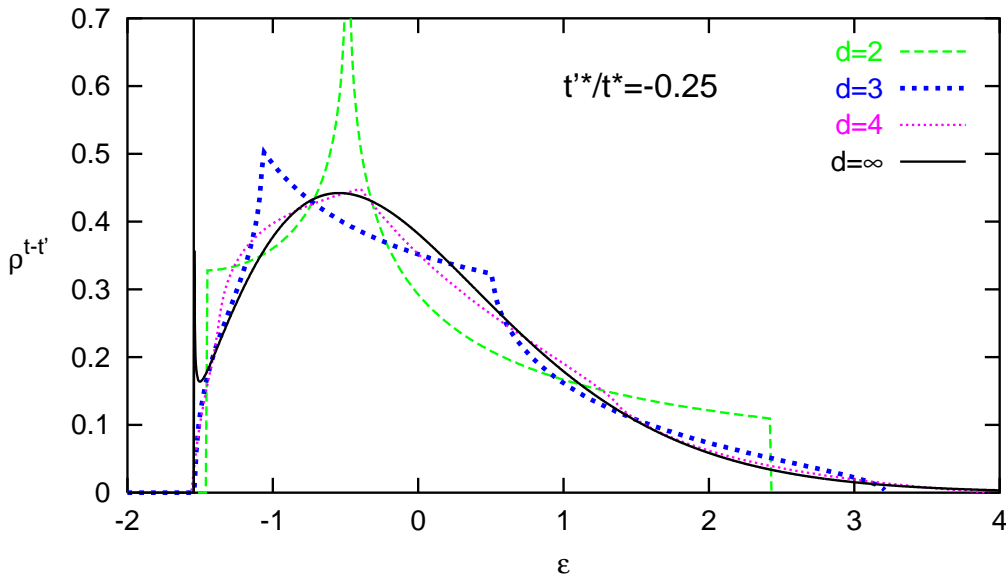
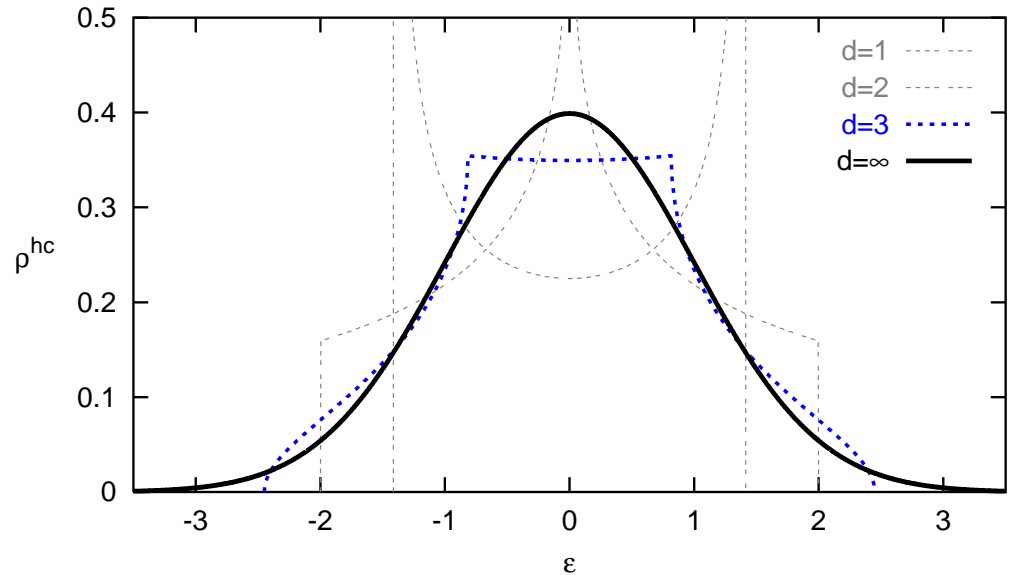
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Inclusion of next-nearest neighbor hopping:

- 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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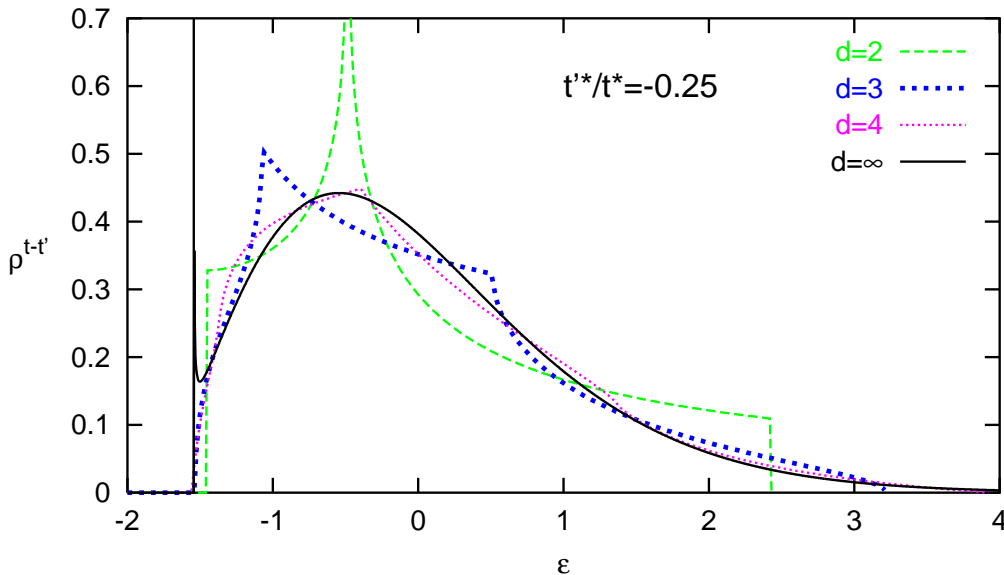
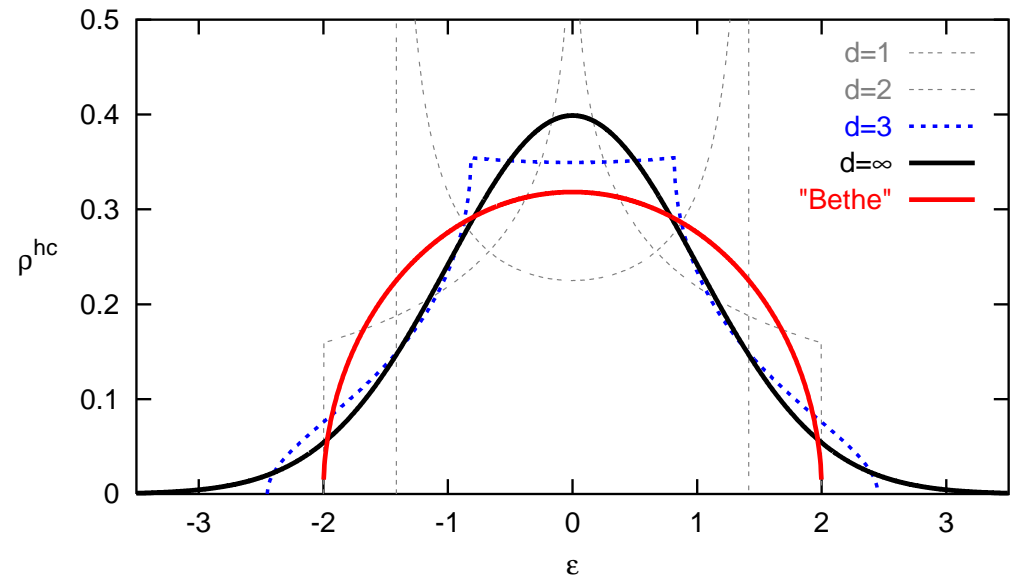
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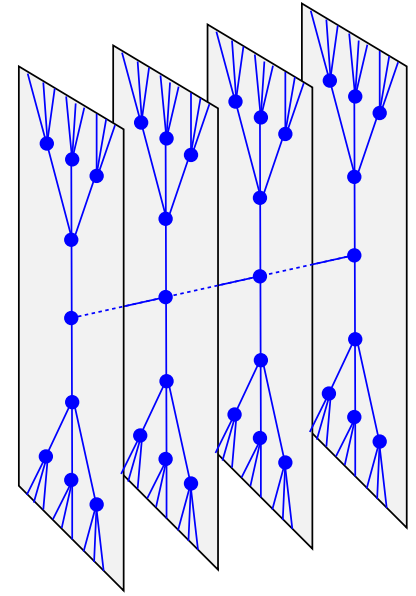
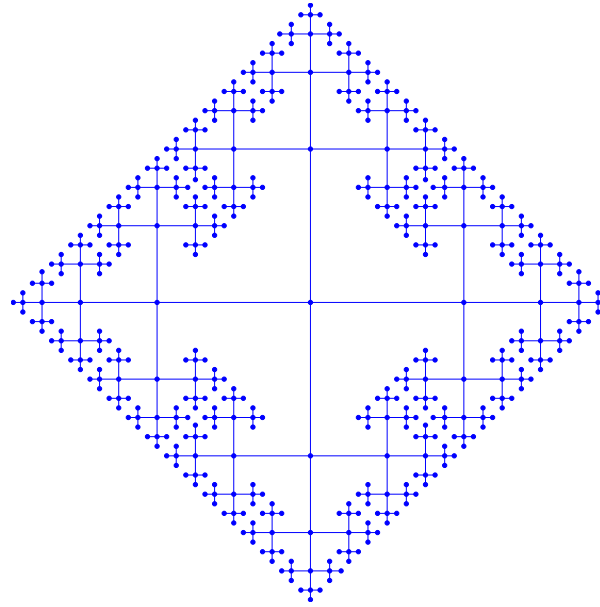
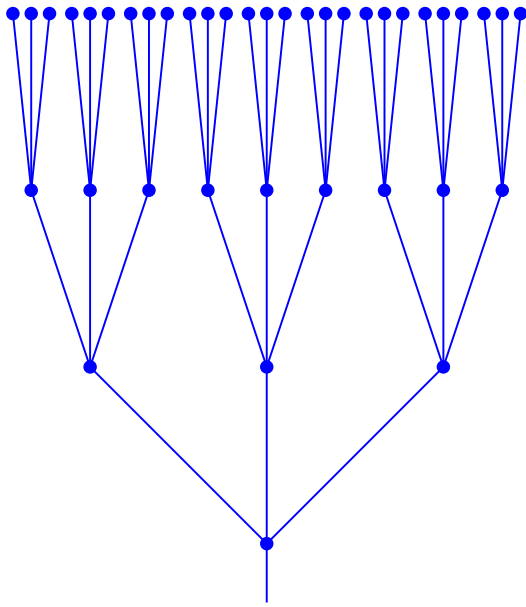
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Pragmatic choice: semi-elliptic "Bethe" DOS



“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 \mathbf{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:

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

In the lattice case: use Peierls construction $t_{ij} = t_{ij}^0 \exp \left[-i \frac{e}{c\hbar} (\mathbf{R}_i - \mathbf{R}_j) \cdot \mathbf{A} \right]$
derive $\hat{\mathbf{j}}$ from $\hat{H}_0 \longrightarrow \hat{H}_0 - \frac{V}{c} \hat{\mathbf{j}} \cdot \mathbf{A} + \mathcal{O}(A^2)$

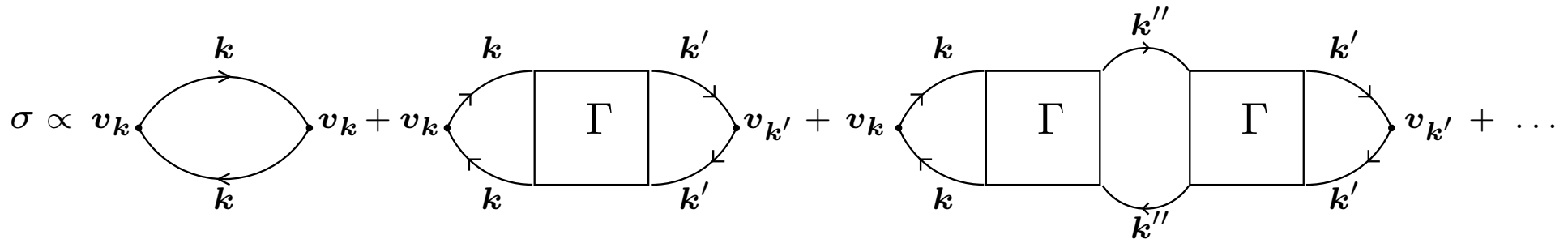
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For a Bravais lattice and a single band: $\hat{\mathbf{j}} = \frac{e}{V\hbar} \sum_{\mathbf{k}, \sigma} \mathbf{v}_{\mathbf{k}} \hat{n}_{\mathbf{k}, \sigma}$ (Fermi velocity $\mathbf{v}_{\mathbf{k}} = \frac{1}{\hbar} \nabla \epsilon_{\mathbf{k}}$)



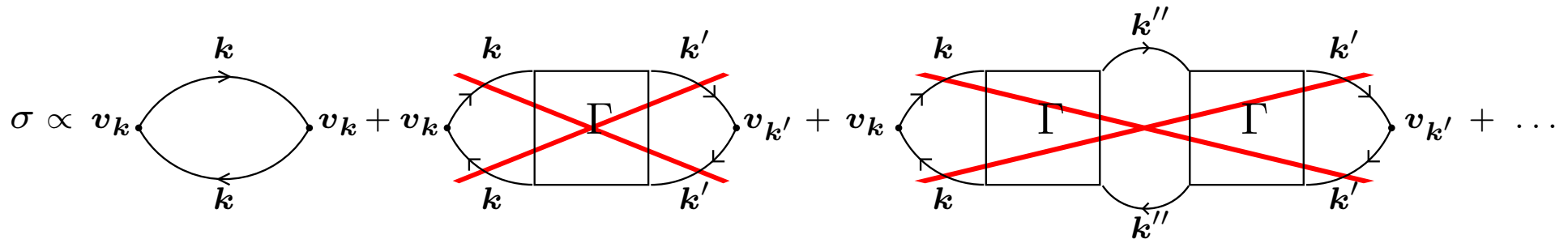
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$d \rightarrow \infty$: Vertex corrections vanish [A. Khurana, Phys. Rev. Lett. **64**, 1990 (1990)]

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

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

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

For hypercubic lattice $(\mathbf{v}_{\mathbf{k}})_x$ effectively constant: $\tilde{\rho}^{\text{hc}}(\epsilon) := \sum_{\alpha} \tilde{\rho}_{\alpha\alpha}^{\text{hc}}(\epsilon) = \rho^{\text{hc}}(\epsilon)$

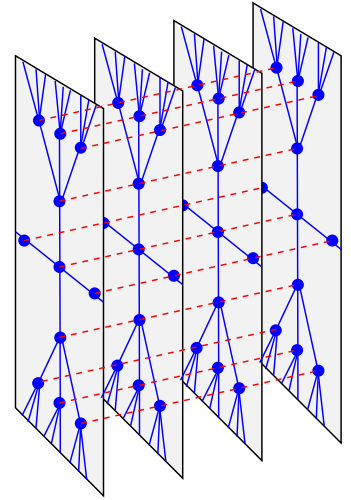
$$\int_0^{\infty} d\omega \sigma_{xx}(\omega) = -\frac{\sigma_0}{4d} \langle \hat{H}_0 \rangle$$

This generalizes to “stacked” lattices with

$$\epsilon_{\mathbf{k}} = \epsilon_{k_x}^x + \epsilon_{\mathbf{k}_{\perp}}^{\perp}, \quad \sqrt{\langle (\epsilon_{k_x}^x - \langle \epsilon_{k_x}^x \rangle)^2 \rangle} = \mathcal{O}(1/d),$$

since then, to leading order,

$$\tilde{\rho}_{xx}(\epsilon) = \frac{1}{N} \sum_{\mathbf{k}} (\mathbf{v}_{\mathbf{k}})_x^2 \delta(\epsilon - \epsilon_{\mathbf{k}_{\perp}}^{\perp}) = \rho(\epsilon) \frac{a_x}{2\pi} \int_{-\pi/a_x}^{\pi/a_x} dk_x (\mathbf{v}_{\mathbf{k}})_x^2 = \rho(\epsilon) \langle (\mathbf{v}_{\mathbf{k}})_x^2 \rangle.$$



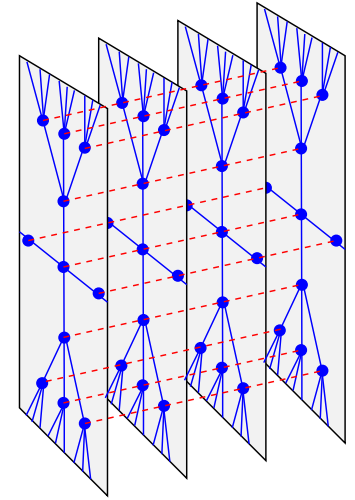
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However, the corresponding generalization of the f -sum rule is useless:

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

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

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

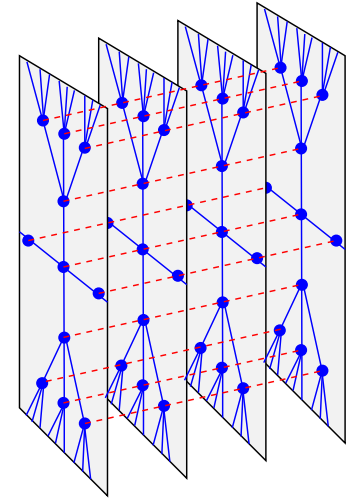
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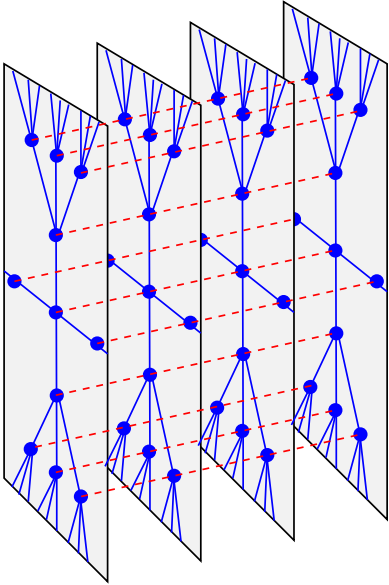
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$$\int_0^{\infty} d\omega \sigma_{xx}(\omega) = \frac{\sigma_0}{4} \left\langle \frac{d}{d\epsilon} \frac{\tilde{\rho}_{xx}(\epsilon)}{\rho(\epsilon)} \right\rangle, \quad \text{where } \langle f(\epsilon) \rangle := \int_{-\infty}^{\infty} d\epsilon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

Previous Approaches for the Bethe Lattice

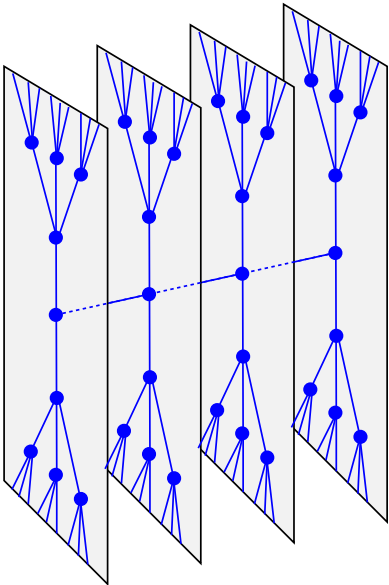


1. Periodically stacked Bethe lattice [G. S. Uhrig and R. Vlaming, *J. Phys. Cond. Matter* **5**, 2561 (1993)]

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

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

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



2. Single-chain layout of Bethe lattice

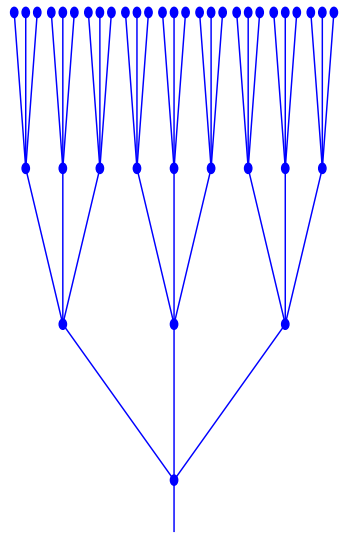
[M. P. H. Stumpf, Ph.D. Thesis, University of Oxford (1999)]

or full offdiagonal disorder

[V. Dobrosavljević and G. Kotliar, *Phys. Rev. Lett.* **71**, 3218 (1993)]

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

- incoherent transport



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

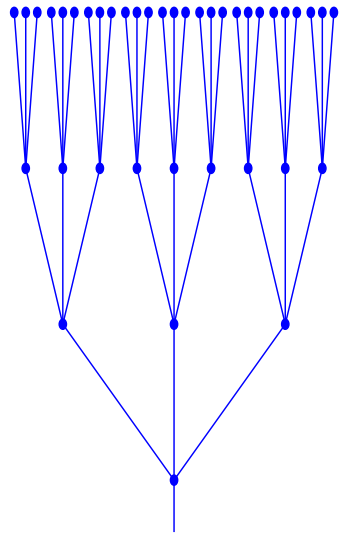
$$\text{Ansatz } |\epsilon\rangle = \sum_x (\gamma_\epsilon)^x \sum_{\alpha_x} |x, \alpha_x\rangle, \quad \gamma_\epsilon = \frac{-\epsilon \pm \sqrt{\epsilon^2 - 4(Z-1)t^2}}{2(Z-1)t}$$

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

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

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

- incomplete derivation, model effectively 1-dimensional



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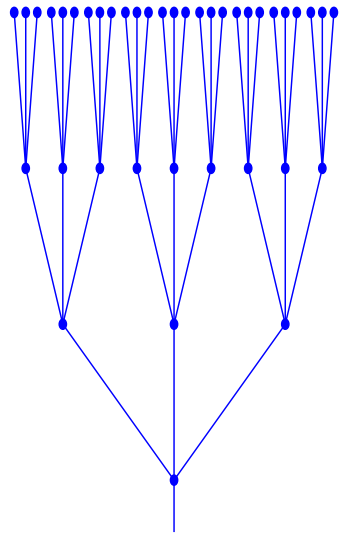
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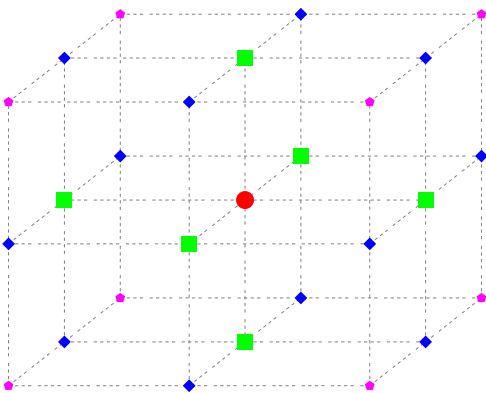
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4. **New:** general dispersion approach

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 $\mathbf{q} \rightarrow 0$)

General Dispersion Formalism

We rewrite the translation-invariant noninteracting Hamiltonian,

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

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

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

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

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

$$\epsilon_D(\mathbf{k}) = t_D \frac{2^D}{D!} \left(\frac{d}{2}\right)^{D/2} B_D(\mathbf{k})$$

$$B_D(\mathbf{k}) = \left(\frac{2}{d}\right)^{D/2} \sum_{\alpha_D \neq \alpha_{D-1} \neq \dots \neq \alpha_1} \cos(k_{\alpha_D}) \cos(k_{\alpha_{D-1}}) \dots \cos(k_{\alpha_1})$$

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

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

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

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

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

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

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

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

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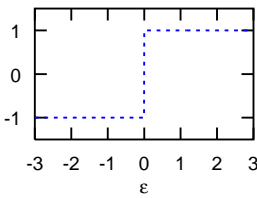
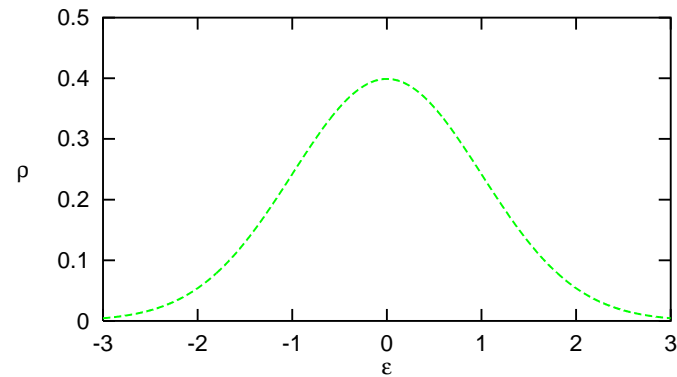
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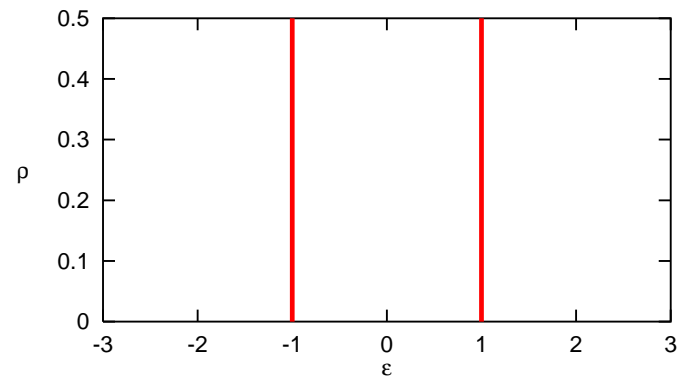
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Choice of **monotonic** transformation function $\mathcal{F}(x)$ implies $\rho(\epsilon) = \frac{1}{\mathcal{F}'(\mathcal{F}^{-1}(\epsilon))} \rho^{\text{hc}}(\mathcal{F}^{-1}(\epsilon))$ and

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



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



Example 1: Flat-band System

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

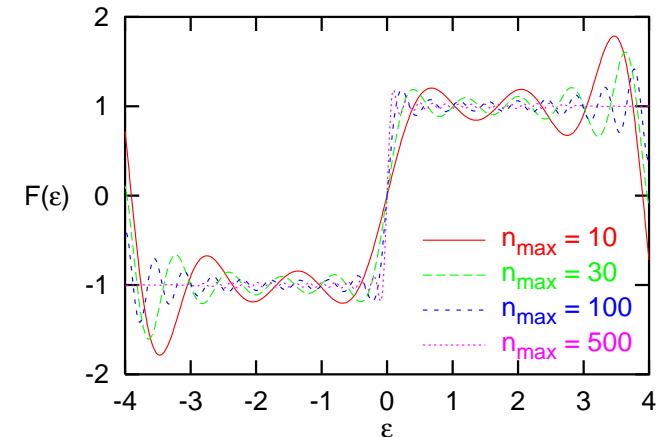
Hopping matrix elements (trivially, $t_{2n}^* = 0$):

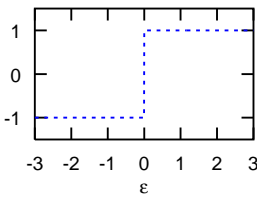
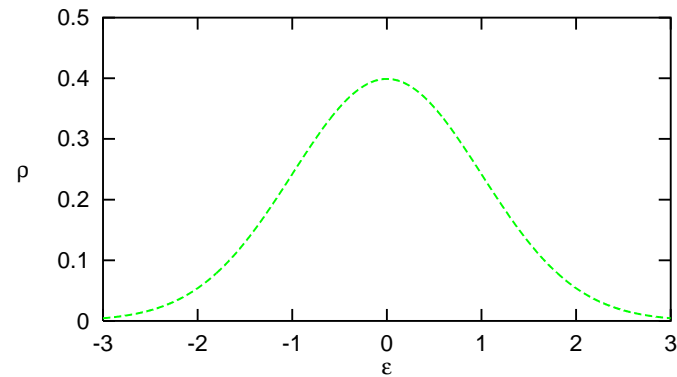
$$t_{2n+1}^* = (-1)^n \sqrt{\frac{2}{\pi}} \frac{(2n-1)!!}{\sqrt{(2n+1)!}} \xrightarrow{n \rightarrow \infty} (-1)^n (\pi n)^{-3/4}$$

asymptotic exponent $-\frac{3}{4}$
 below threshold value $-\frac{1}{2}$
 required for finite variance

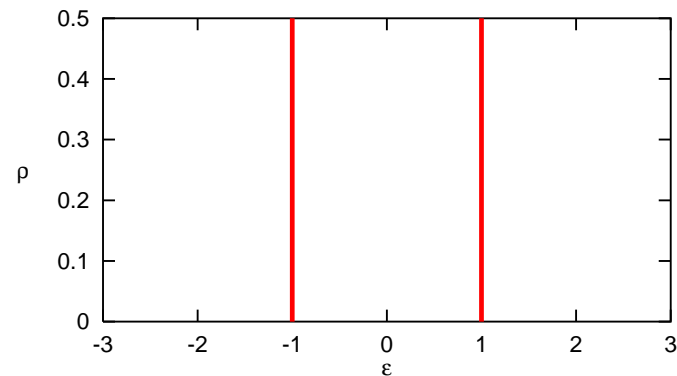
$$\langle \epsilon^2(\mathbf{k}) \rangle = \sum_D t_D^*{}^2$$

slow convergence of \mathcal{F}





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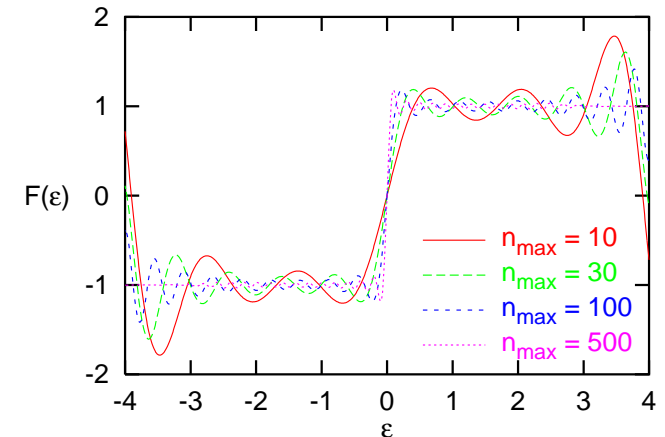
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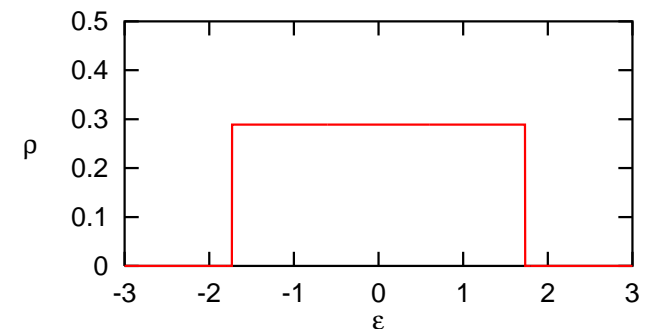


Example 2: constant DOS

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

decay of t_D^* is already exponential

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

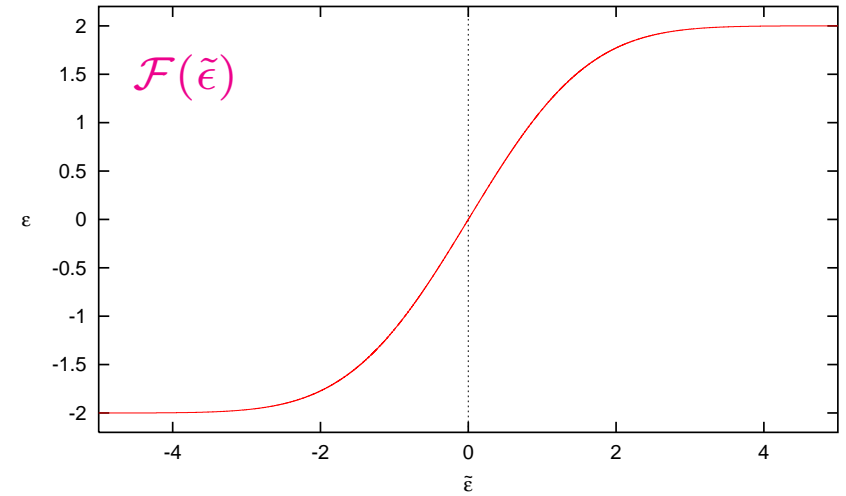


Redefinition of the Bethe Lattice

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

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

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



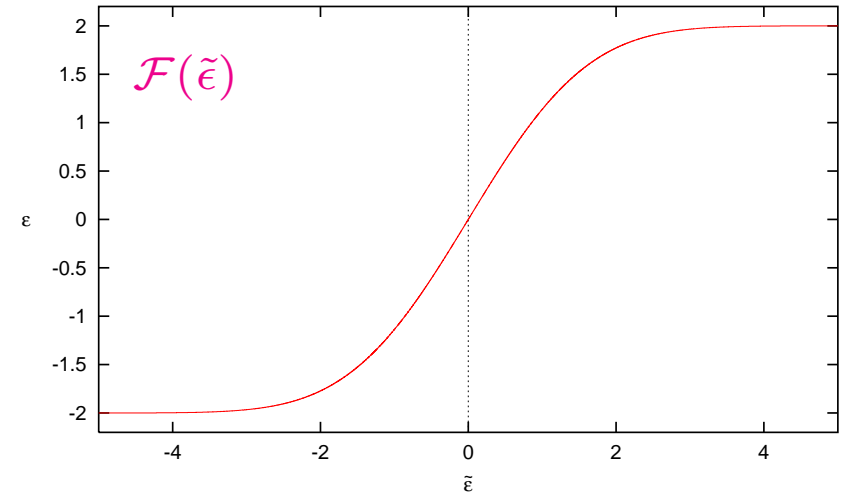
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numerical integration $\rightsquigarrow t_D^*$



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1	0.98731	0.974773
3	-0.15353	0.998345
5	0.03893	0.999861
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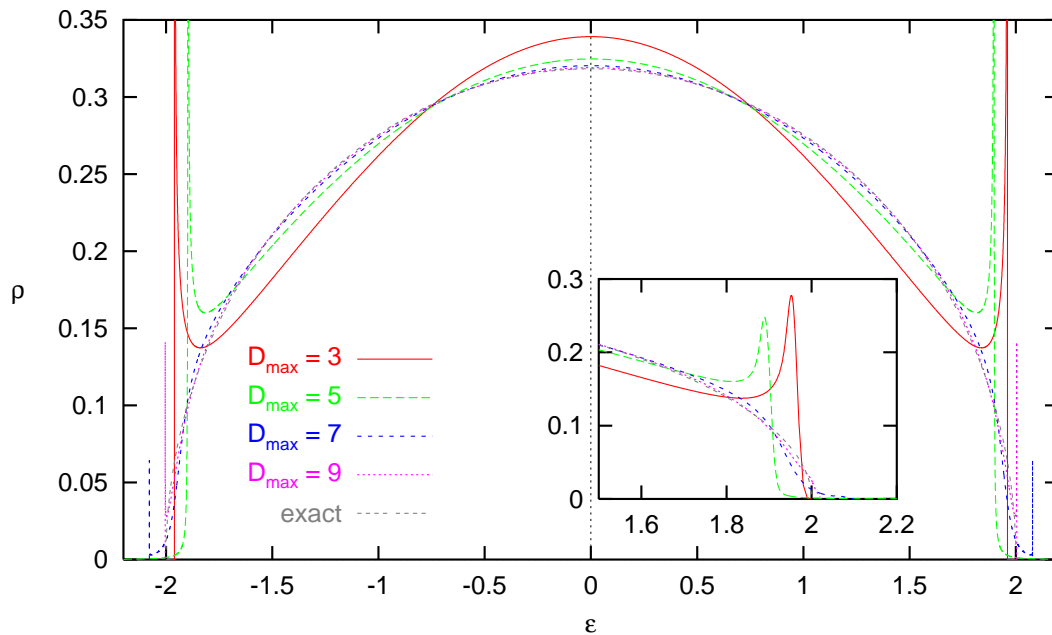
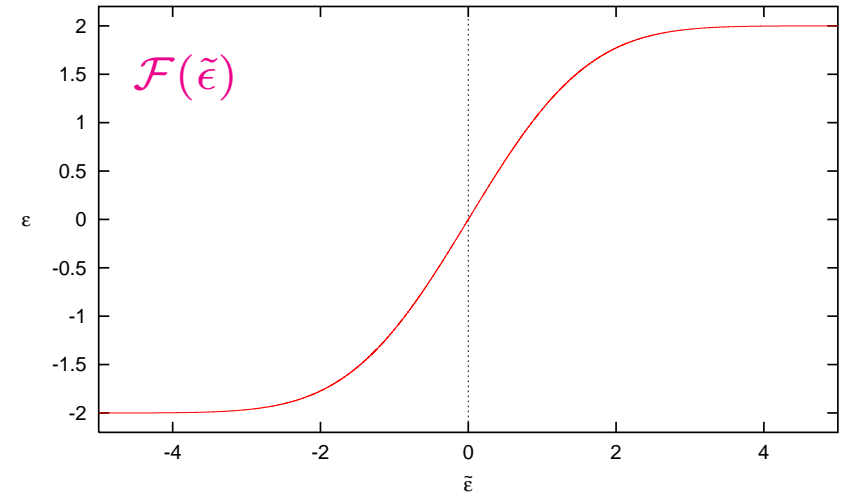
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numerical integration $\rightsquigarrow t_D^*$

fast convergence with maximal hopping distance D_{\max}

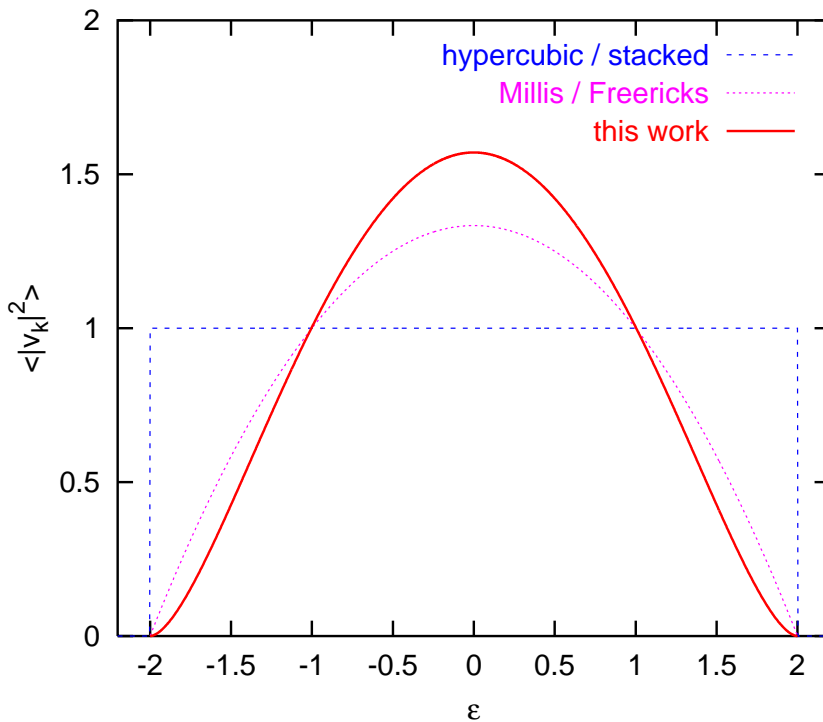


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Chain rule yields Fermi velocity in general dispersion formalism: $\mathbf{v}_{\mathbf{k}} = \mathcal{F}'(\mathcal{F}^{-1}(\epsilon))\mathbf{v}_{\mathbf{k}}^{\text{hc}}$.

Specifically, for Bethe semi-elliptic DOS:

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

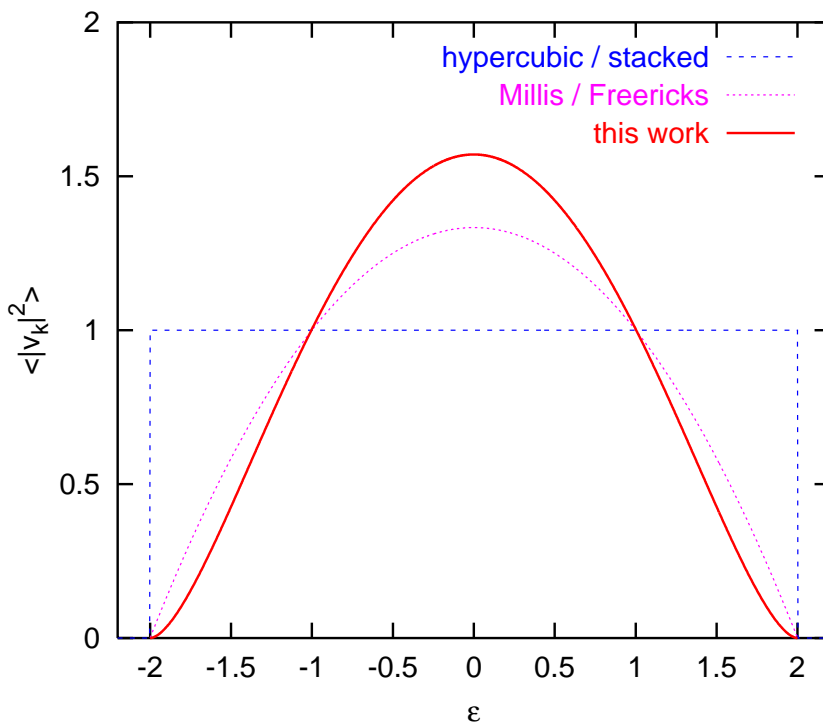


- squared Fermi velocity vanishes at the band edges as required physically
- maximal contribution to transport from states at band center
- effect even stronger than found/assumed by Freericks and Millis
- lattice input for other transport properties can be derived analogously

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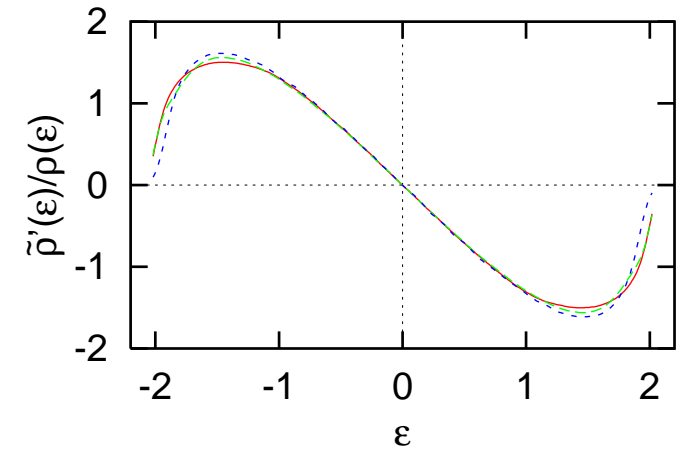
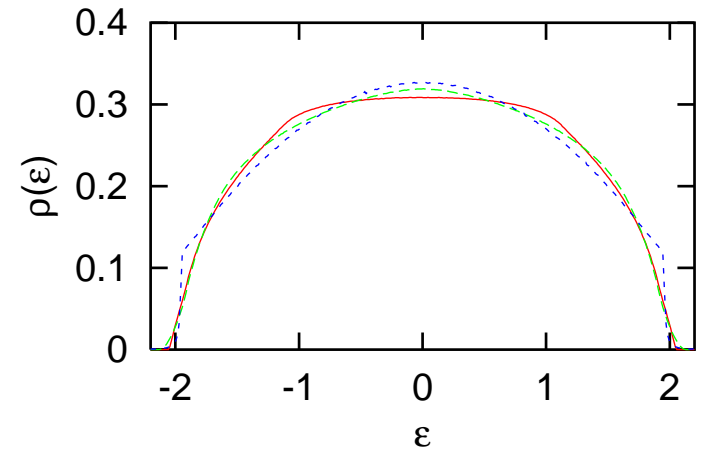
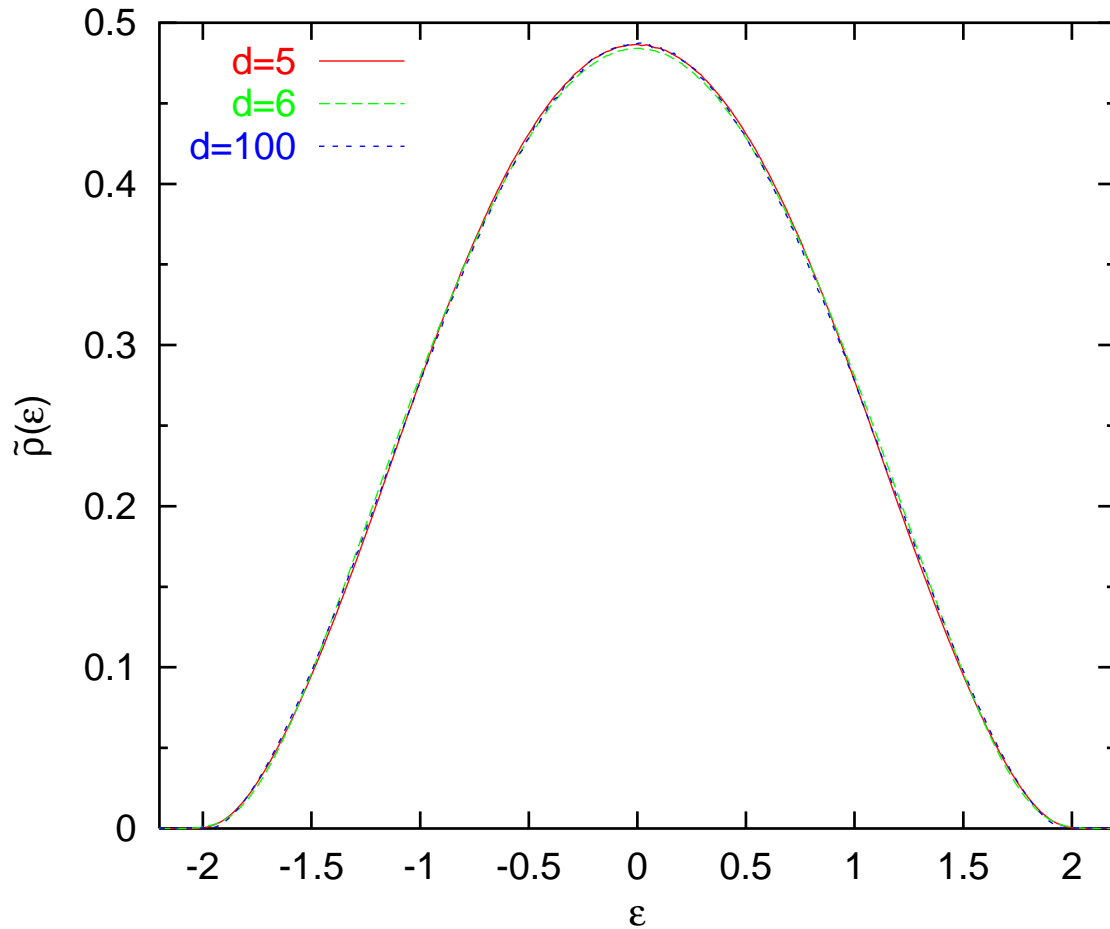
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f-sum rule:
$$\int_0^\infty d\omega \sigma_{xx}(\omega) = \frac{\sigma_0}{4d} \left\langle \frac{\tilde{\rho}'(\epsilon)}{\rho(\epsilon)} \right\rangle = \frac{\sigma_0}{4d} \left\langle \left[\mathcal{F}''(\mathcal{F}^{-1}(\epsilon)) - \mathcal{F}^{-1}(\epsilon)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

Test for robustness: finite hopping range and finite dimensionality

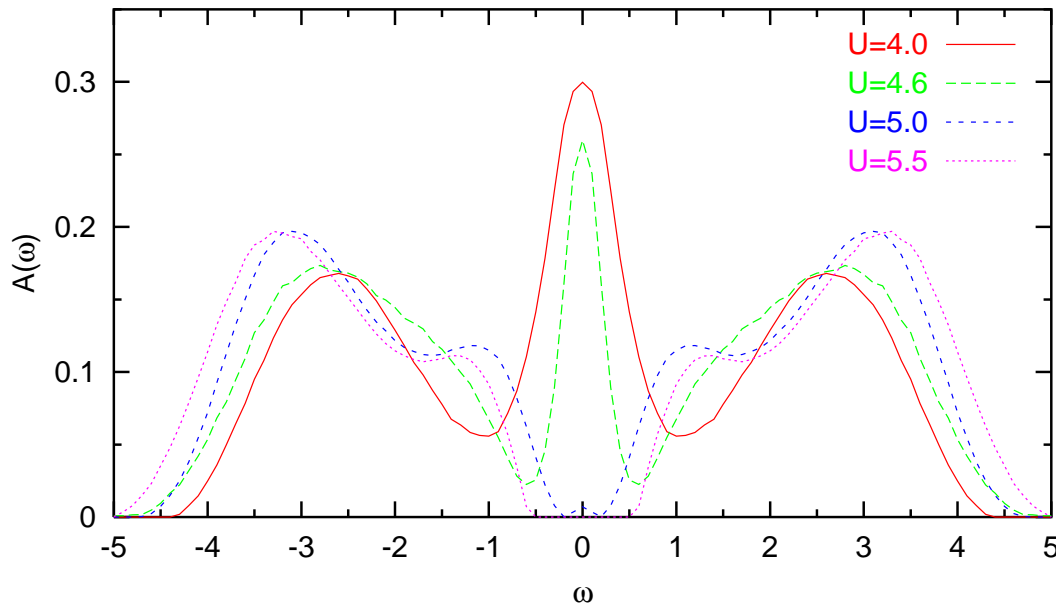
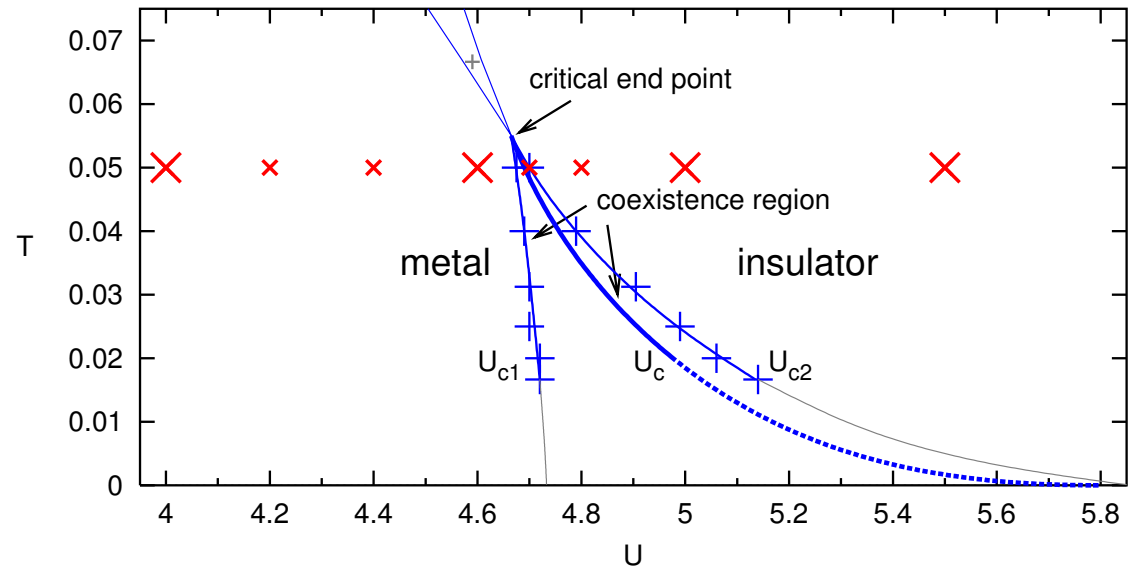


Restriction to 5th nearest neighbor hopping leads to a slight suppression of $\tilde{\rho}(\epsilon)$

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

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

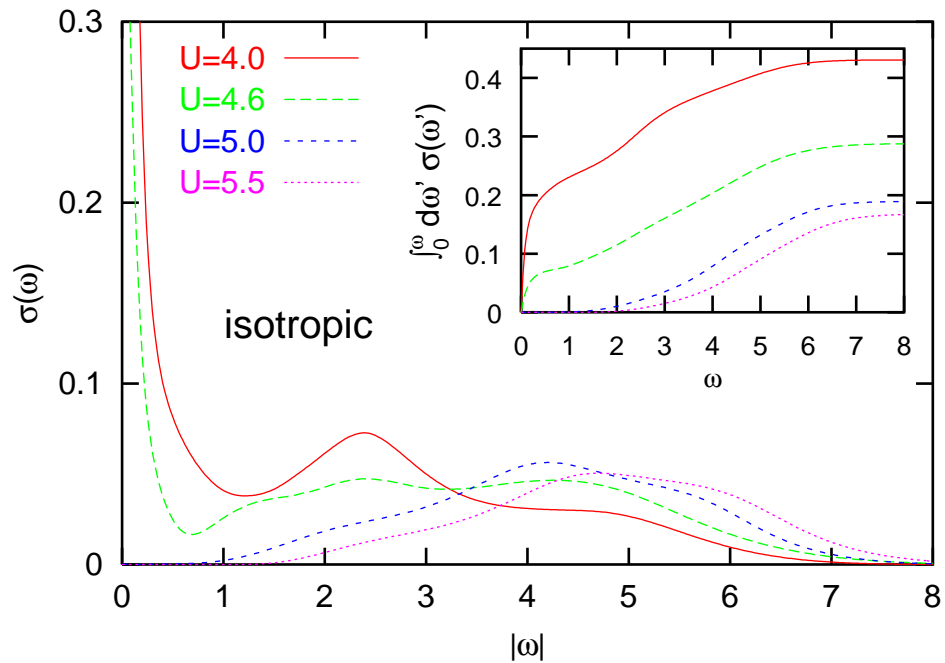
Metal-insulator transition region for
 $4.0 \leq U \leq 5.5$ and $T = 0.05$,
 just below $T^* \approx 0.055$



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

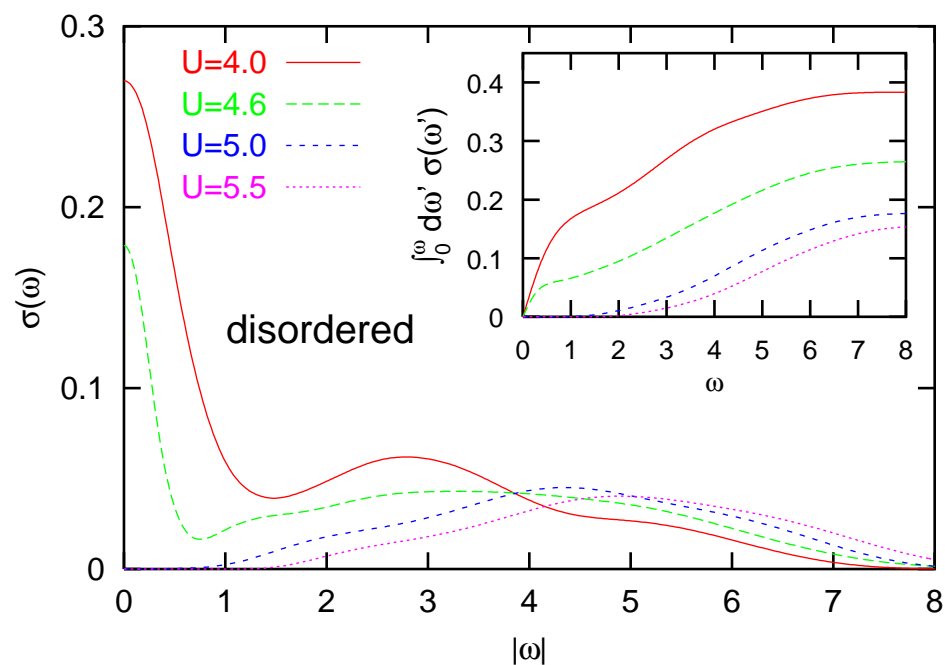
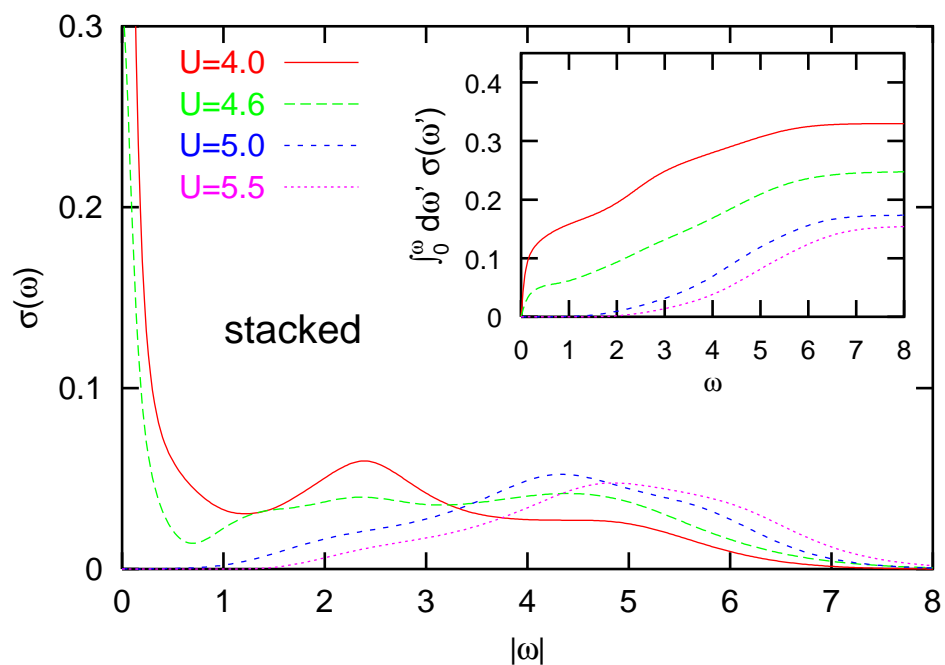
MEM using flat default model

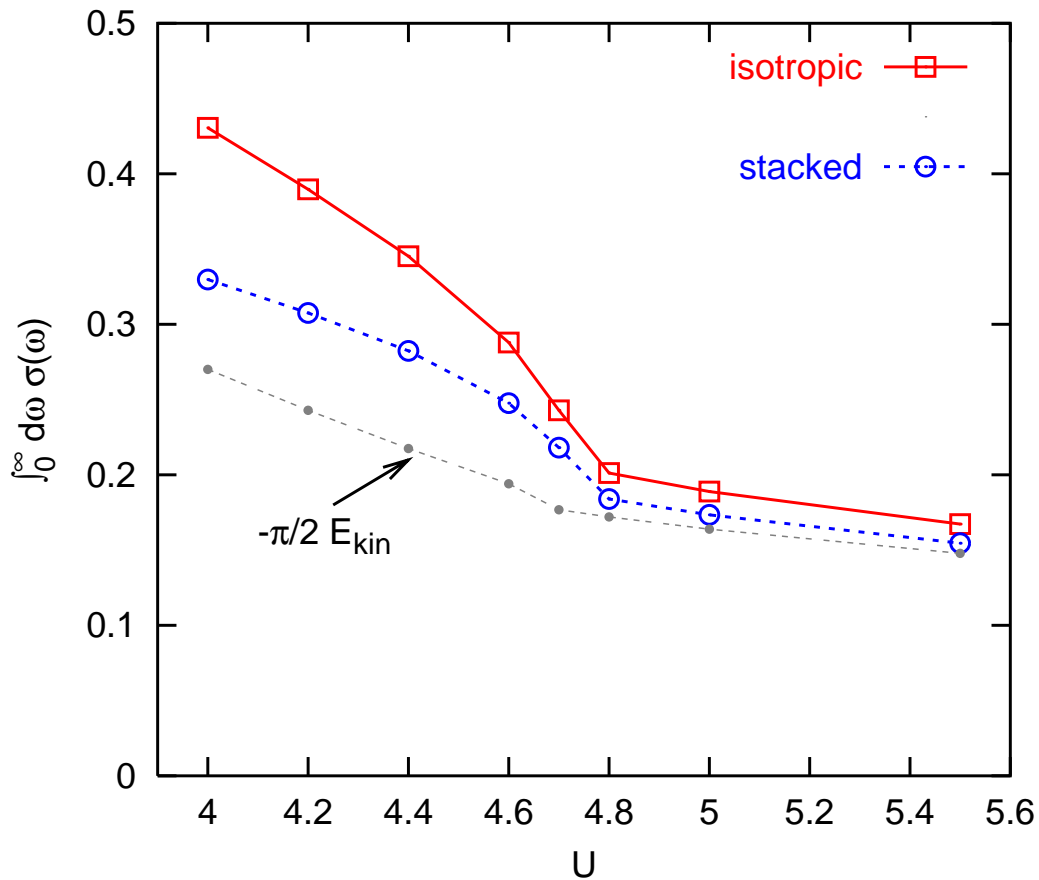
- good Luttinger pinning for $U \lesssim 4.4$
- quasiparticle peak disappears at the transition ($U \approx 4.7$)
- gap opens for $U \gtrsim 5.0$



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



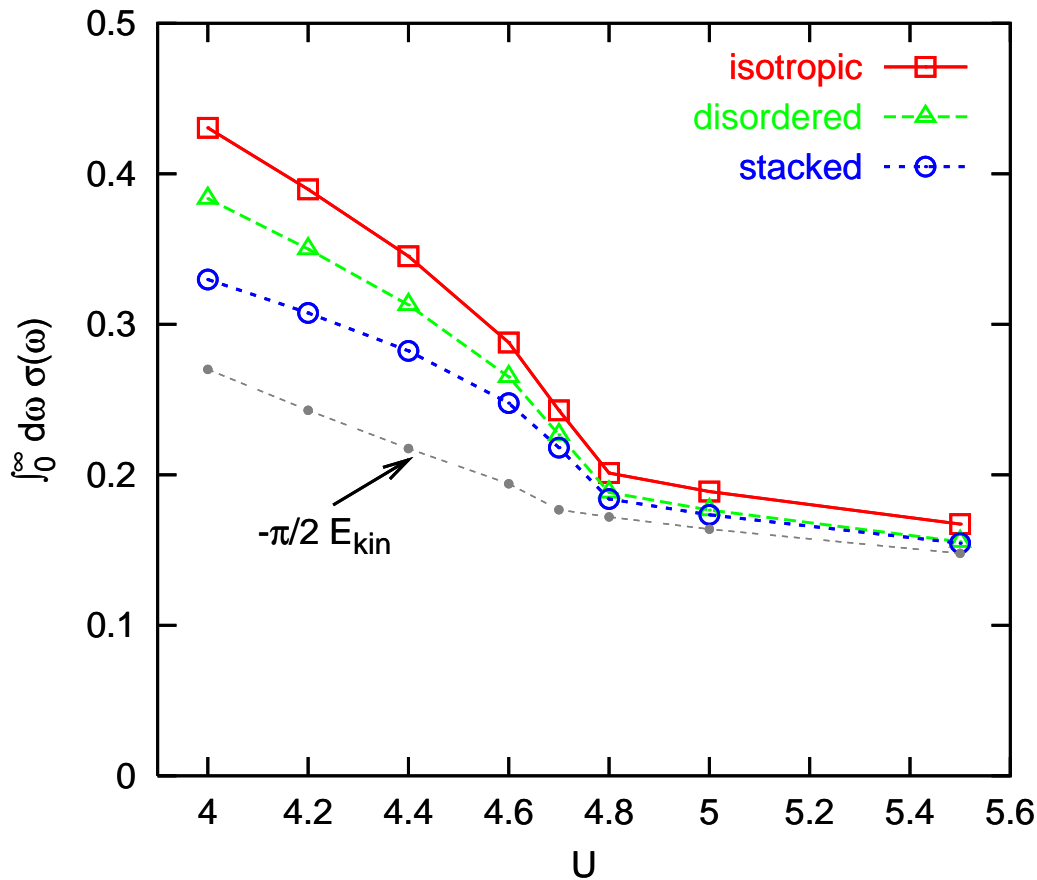


f -sum generally larger for the isotropic case

effect 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

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



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disordered / single-chain case in-between
 with respect to 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 with sharp (3d like) band edges in $d \rightarrow \infty$
- 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

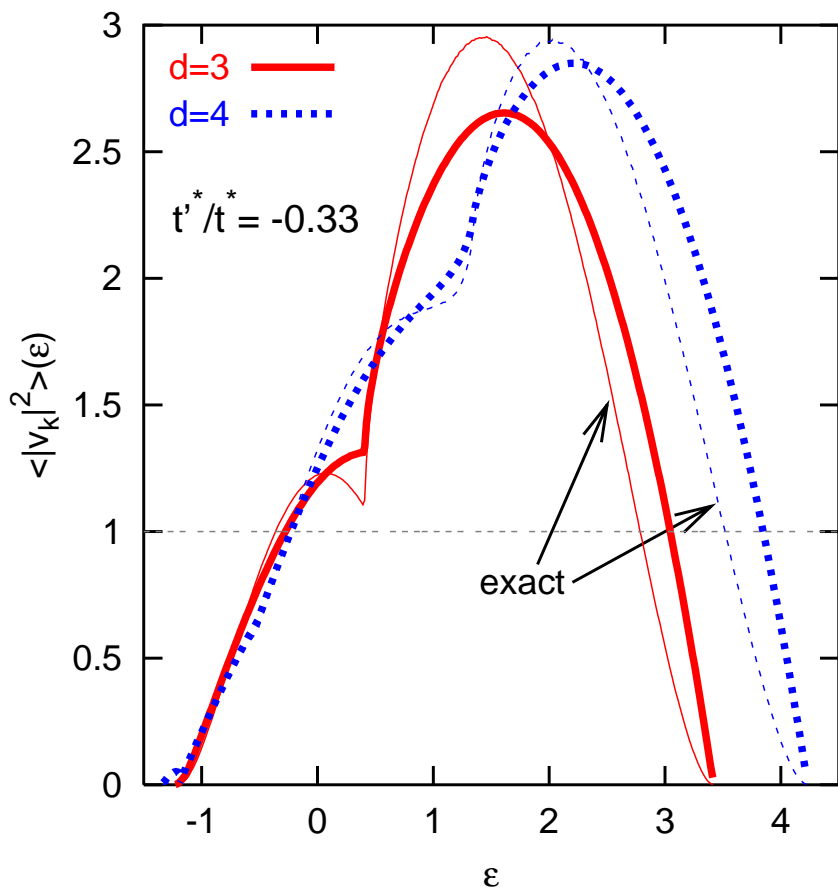
numerical results for $\sigma(\omega)$ based on high-precision QMC/MEM spectra

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 $\text{La}_{1-x}\text{Sr}_x\text{TiO}_3$ based on LDA data

