Optical Conductivity of Strongly Correlated Electron Systems in High Dimensions

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Outline

Introduction

Optical Conductivity near a MIT for $d \to \infty$

General Dispersion Formalism

Numerical QMC/MEM Results for Half-filled Hubbard Model

Conclusion

Introduction

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

linear response
homogeneous system
limit $\boldsymbol{q} \to 0$

$$\left.\begin{array}{c}\text{linear response}\\ \text{homogeneous system}\\ \text{limit } \boldsymbol{q}\to 0\end{array}\right\} \Rightarrow \qquad J_\alpha(\omega) = \sum_{\beta=1}^{d} \sigma_{\alpha\beta}(\omega)\, E_\beta(\omega)$$

specular reflectivity $r(\omega) = \left| \frac{1-\sqrt{\epsilon(\omega)}}{1+\sqrt{\epsilon(\omega)}} \right|^2 \xrightarrow{\text{K-K}}$ dielectric function $\epsilon(\omega) = 1 + \frac{4\pi i}{\omega} \sigma(\omega)$

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The f-sum rules

bounded absorption spectrum:

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

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

$$\Longrightarrow \qquad \int_0^\infty \mathrm{d}\omega\ \mathrm{Re}\, \sigma(\omega) = \frac{\omega_{\mathrm{p}}^2}{8}$$

Optical f-sum rule

Full universal f-sum rule: $\omega_{\mathrm{p}}^2 = \dfrac{4\pi n e^2}{m}$ (independent of T, interactions etc.)

Kubo formalism

For continuum systems:

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

Lattice case: $\hat{H}_0 = \hat{K} + \hat{H}_{\text{int}} \equiv \sum_{ij,\sigma} t^0_{ij}\, \hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} + \hat{H}_{\text{int}}\{\hat{n}_{i\sigma}\}$

Peierls construction $t_{ij} = t^0_{ij} \exp\left[-i \frac{e}{c\hbar} (\boldsymbol{R}_i - \boldsymbol{R}_j) \cdot \boldsymbol{A}\right]$

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

Bravais lattice, one-band: $\hat{K} = \frac{1}{V} \sum_{\boldsymbol{k},\sigma} \epsilon_{\boldsymbol{k}}\, \hat{n}_{\boldsymbol{k},\sigma}$, $\hat{\boldsymbol{\jmath}} = \frac{e}{V\hbar} \sum_{\boldsymbol{k},\sigma} \boldsymbol{v}_{\boldsymbol{k}}\, \hat{n}_{\boldsymbol{k},\sigma}$ $\left(\boldsymbol{v}_{\boldsymbol{k}} = \frac{1}{\hbar} \nabla \epsilon_{\boldsymbol{k}}\right)$

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Hypercubic lattice, NN hopping:

$$\hat{K} = \sum_{\alpha=1}^{d} \hat{K}_\alpha\,;\;\; \hat{K}_\alpha = \frac{2}{N}\,\mathrm{Re} \sum_{i\sigma} \hat{c}_{\boldsymbol{R}_i+\boldsymbol{e}_\alpha}^\dagger \hat{c}_{\boldsymbol{R}_i}\,;\;\; \hat{j}_\alpha = \frac{e}{\hbar}\frac{2}{N}\,\mathrm{Im} \sum_{i\sigma} \hat{c}_{\boldsymbol{R}_i+\boldsymbol{e}_\alpha}^\dagger \hat{c}_{\boldsymbol{R}_i}$$

$$\int_0^\infty \mathrm{d}\omega\, \sigma_{\alpha\alpha}(\omega) = -\frac{\pi}{2}\frac{e^2 a^2}{V\hbar^2}\langle \hat{K}_\alpha \rangle = -\frac{\pi}{2}\frac{e^2 a^2}{V\hbar^2}\frac{1}{d}\langle \hat{K} \rangle \;\equiv\; -\frac{\sigma_0}{4d}\langle \epsilon \rangle$$

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Hypercubic lattice, NN hopping:

$$\hat{K} \neq \sum_{\alpha=1}^d \hat{K}_\alpha\, ;\; \hat{K}_\alpha = \frac{2}{N}\,\text{Re}\sum_{i\sigma} \hat{c}_{\boldsymbol{R}_i+\boldsymbol{e}_\alpha}^\dagger \hat{c}_{\boldsymbol{R}_i}\, ;\; \hat{\jmath}_\alpha = \frac{e}{\hbar}\frac{2}{N}\,\text{Im}\sum_{i\sigma} \hat{c}_{\boldsymbol{R}_i+\boldsymbol{e}_\alpha}^\dagger \hat{c}_{\boldsymbol{R}_i}$$

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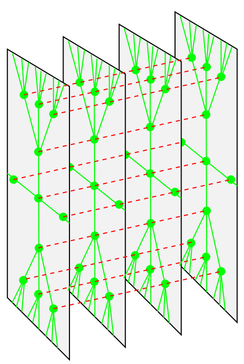
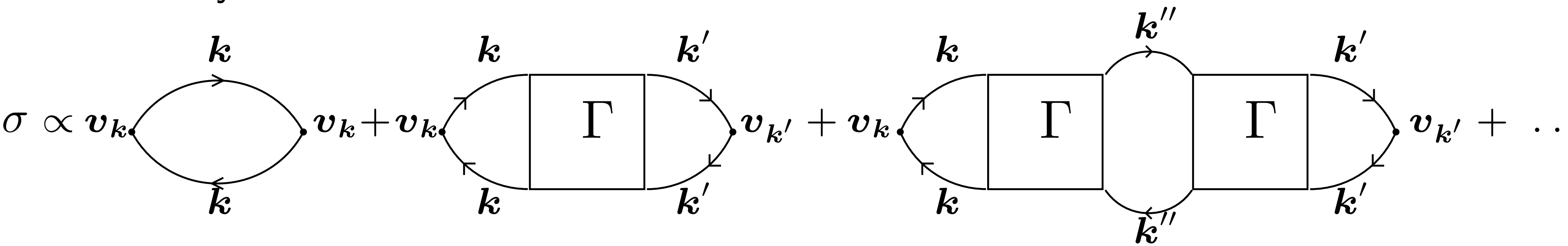


stacked

DMFT Treatment of the Optical Conductivity

Conductivity on Bravais lattice:



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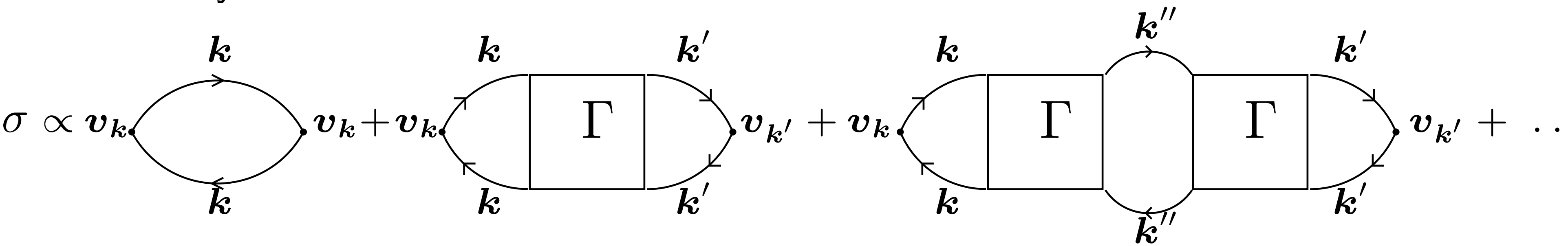

DMFT: limit $d \to \infty$ / $Z \to \infty$: scaling $t \propto 1/\sqrt{Z}$, $\Sigma(\boldsymbol{k}, \omega) \to \Sigma(\omega)$

local properties depend on lattice only via $\rho(\epsilon) := \frac{1}{N} \sum_{\boldsymbol{k}} \delta(\epsilon - \epsilon_{\boldsymbol{k}})$

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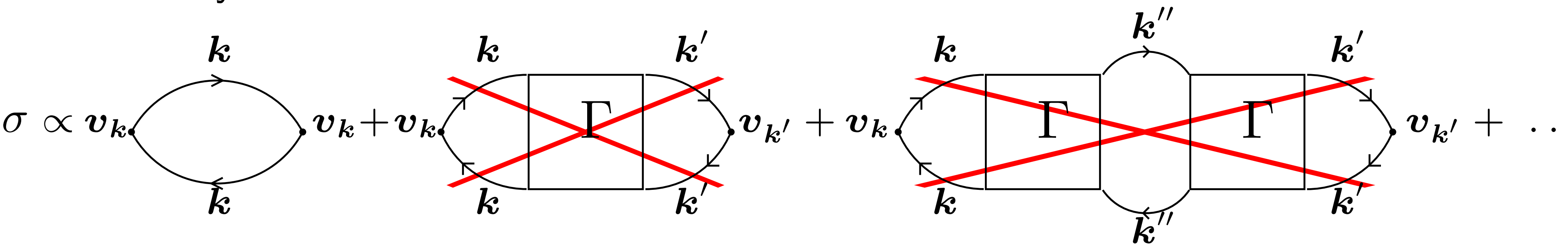

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$d \to \infty$: Vertex corrections vanish [Khurana, PRL **64**, 1990 (1990)]

$\boldsymbol{k}$ sum $\to$ ϵ integral [Pruschke, Cox, and Jarrell, PRB **47**, 3553 (1993)]

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

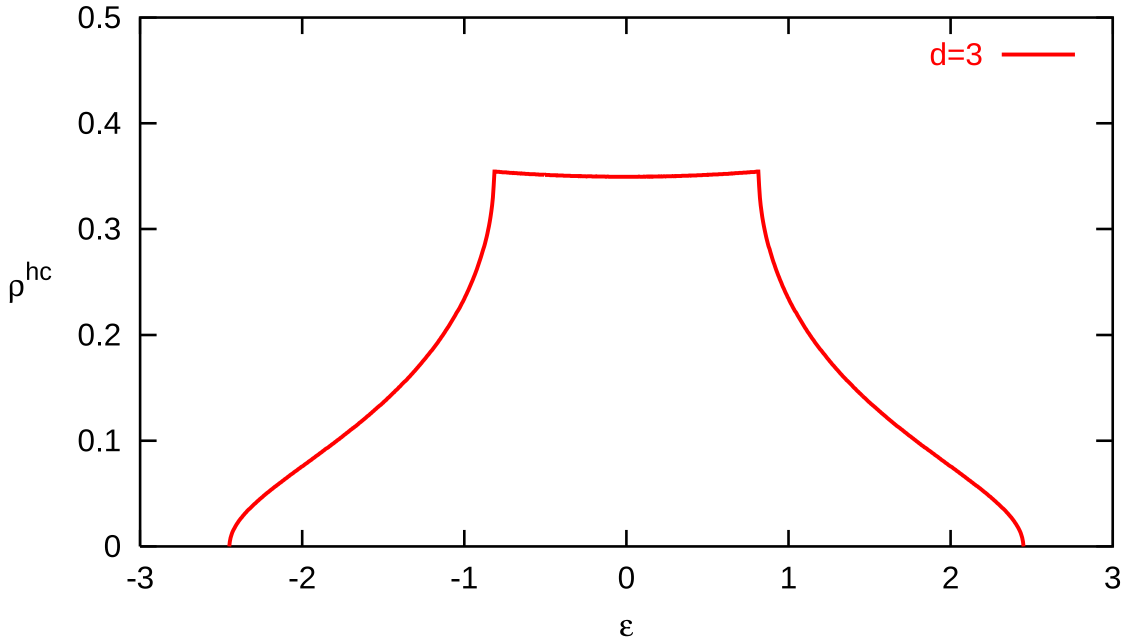
$$\sigma_0 := \frac{2\pi e^2}{\hbar^2}\frac{N}{V}, \quad \tilde{\rho}_{xx}(\epsilon) := \frac{1}{N}\sum_{\boldsymbol{k}} (\boldsymbol{v}_{\boldsymbol{k}})_x^2 \, \delta(\epsilon - \epsilon_{\boldsymbol{k}}), \quad A_\epsilon(\omega) := -\frac{1}{\pi} \, \mathrm{Im} \, \frac{1}{\omega - \epsilon - \Sigma(\omega)}$$

Optical Conductivity Near an MIT for $d \to \infty$

Lattice and Density of States

Nearest-neighbor (NN) hopping on hypercubic (hc) lattice:

$d = 3$: square-root band edges



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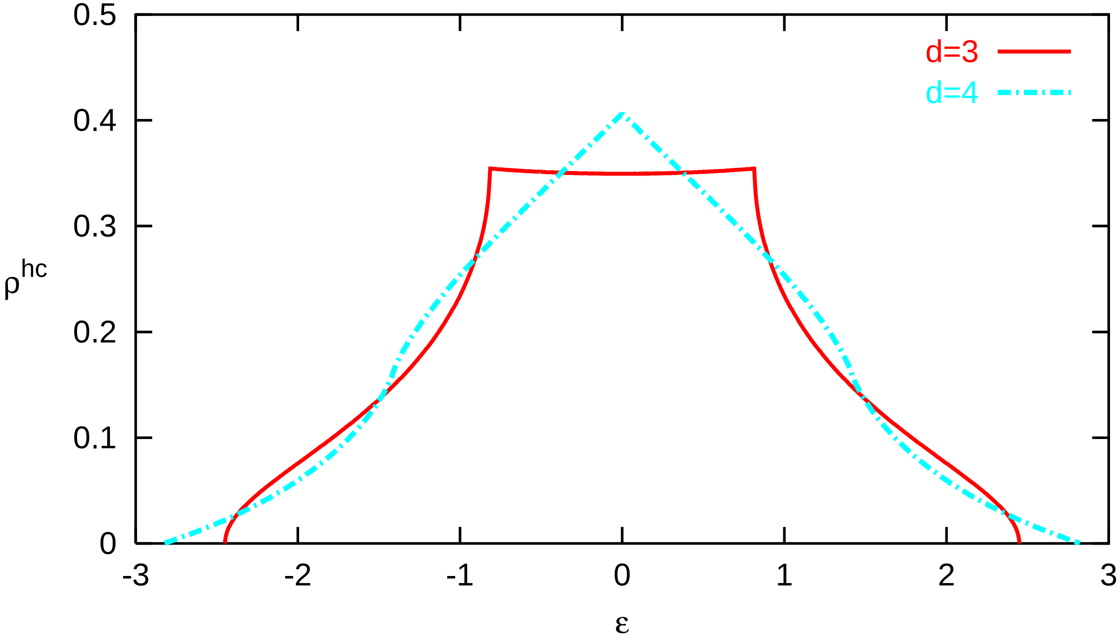

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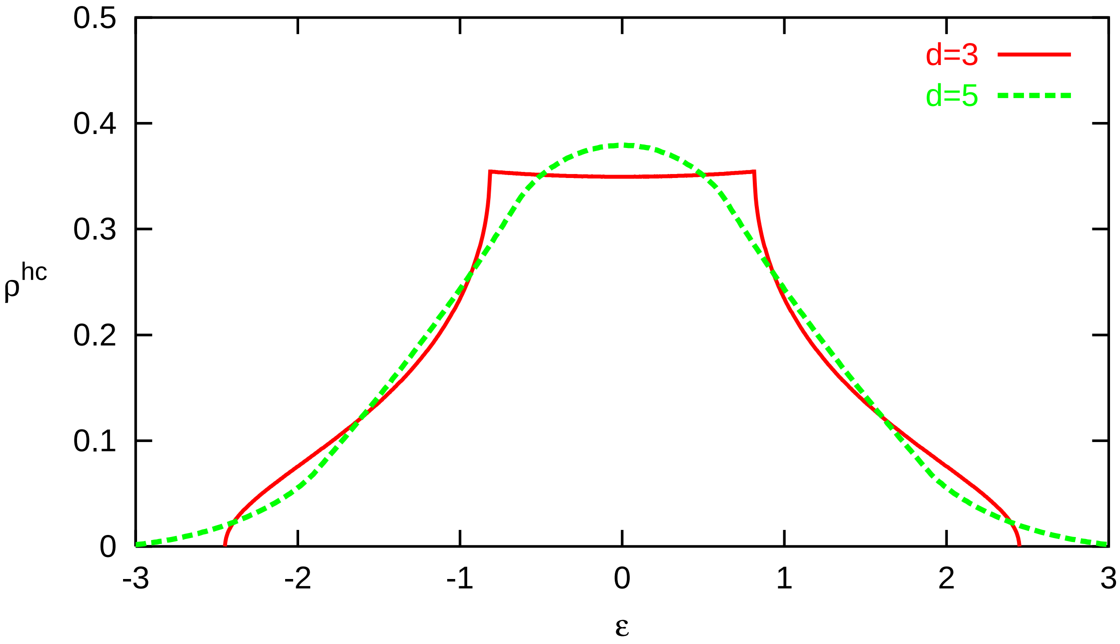

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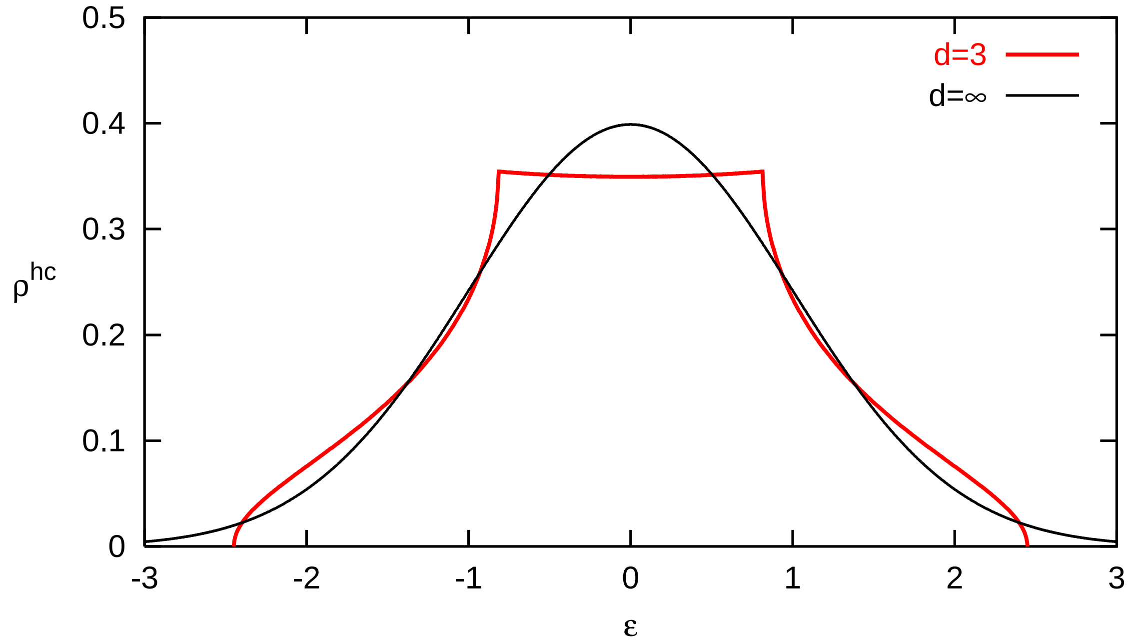
$d \to \infty$: no band edges



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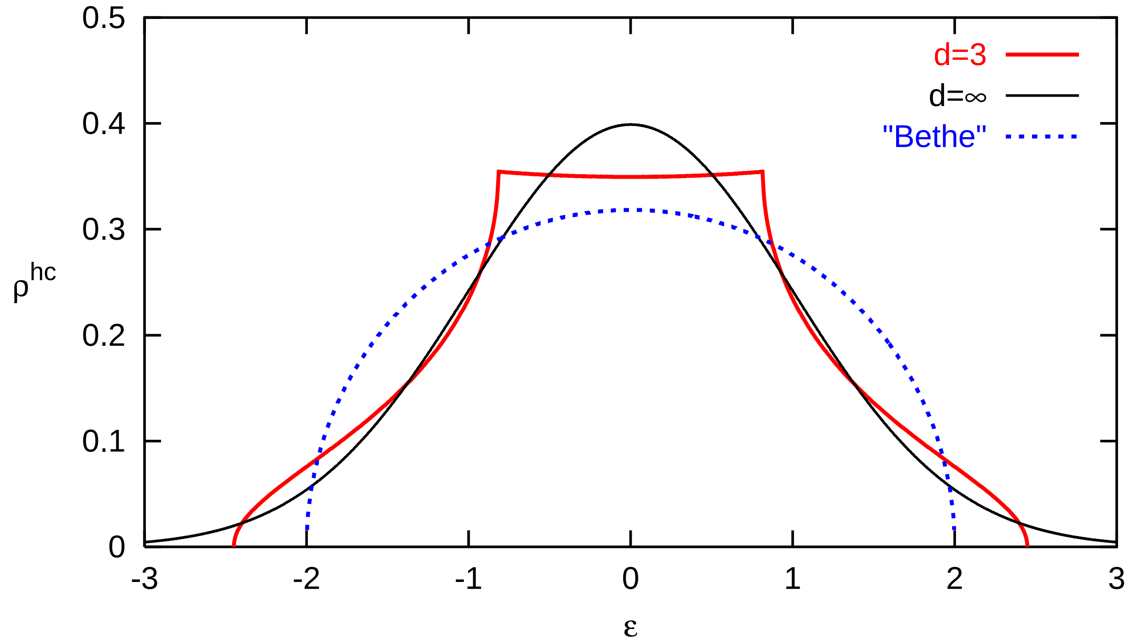

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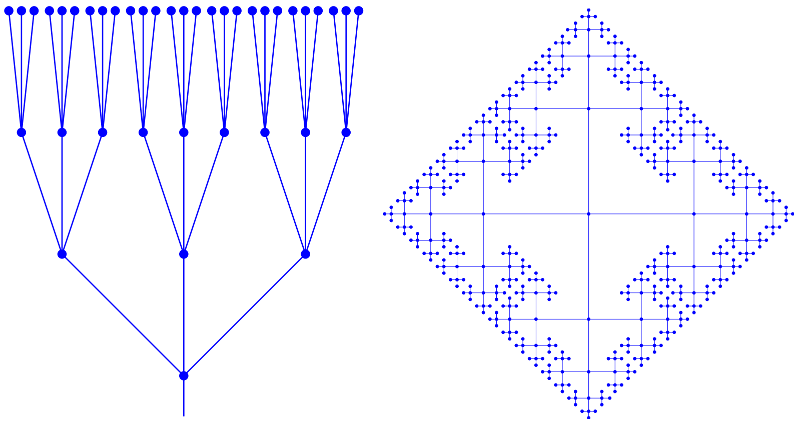

transport properties of Bethe lattice a priori undefined

Bethe-"lattice" (Z=4)

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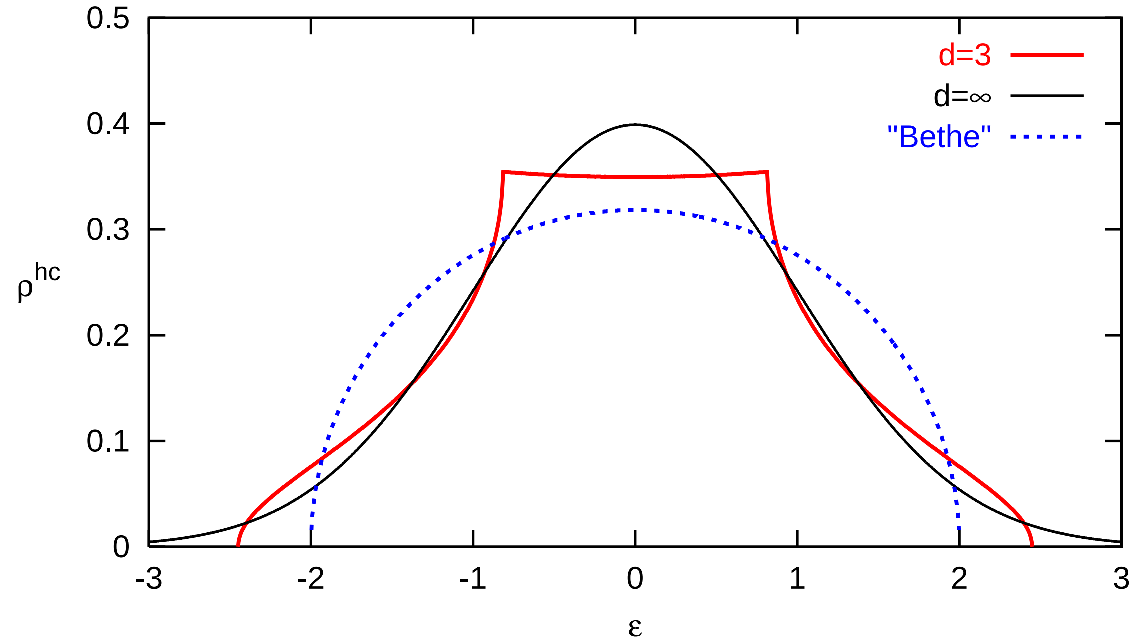

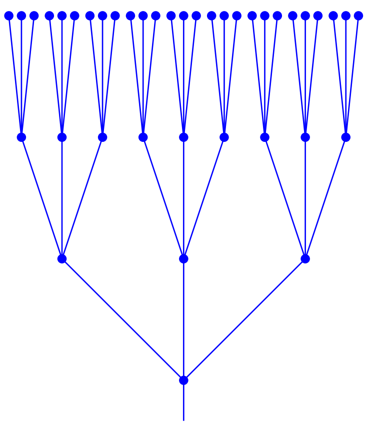

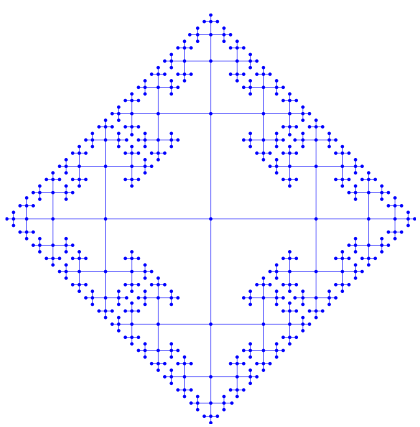

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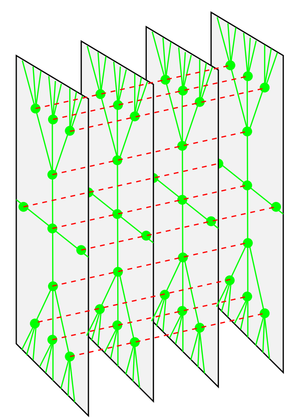
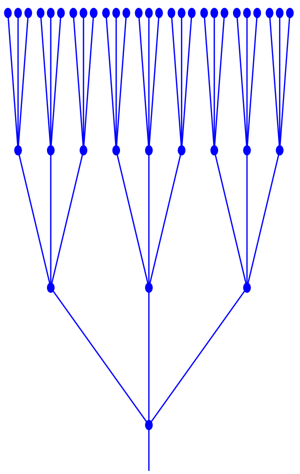


transport properties of Bethe lattice a priori undefined

previously coherent definition of $\sigma(\omega)$ only for periodically continued lattice: anisotropic

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

Optical conductivity for the Bethe lattice



Tree level picture [Chung and Freericks, PRB **57**, 11955 (1998)]

Ansatz for $|\epsilon\rangle$ $\Rightarrow$ $\hat{K}\,|\epsilon\rangle = \epsilon\,|\epsilon\rangle, \quad \hat{j}\,|\epsilon\rangle = \langle v_{\boldsymbol{k}}\rangle(\epsilon)\; e\,|\epsilon\rangle$

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

But: incomplete set of states $\rightsquigarrow$ $\rho(\epsilon) = \frac{1}{\pi\sqrt{4-\epsilon^2}}$: 1-dimensional

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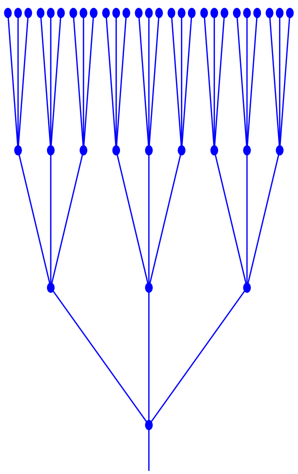

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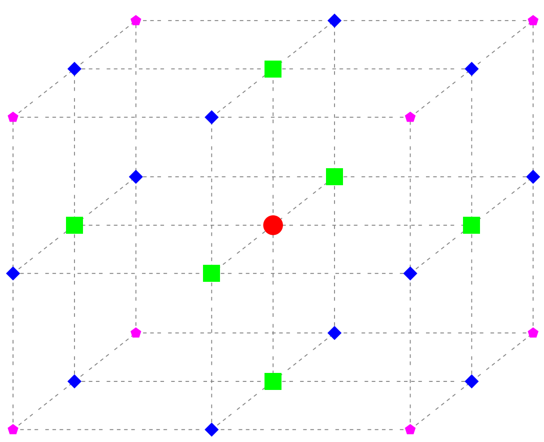

New: general dispersion approach

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

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

General Dispersion Formalism

For translation-invariant hopping: $\hat{K} = \sum_{i,\sigma} \sum_{\boldsymbol{\tau}} t_{\boldsymbol{\tau}} \, \hat{c}^{\dagger}_{\boldsymbol{R}_i+\boldsymbol{\tau},\sigma} \, \hat{c}_{\boldsymbol{R}_i \, \sigma} = \sum_{\boldsymbol{k},\sigma} \epsilon(\boldsymbol{k}) \hat{n}_{\boldsymbol{k}\sigma}$

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

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

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For $d \to \infty$, almost all vectors with $\|\boldsymbol{\tau}\| = D$ have form $\boldsymbol{\tau} = \sum_{i=1}^{D} \boldsymbol{e}_{\alpha_i}$ with $\alpha_i \neq \alpha_j$.

$\overset{\text{isotropy}}{\Longrightarrow}$

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

Functions $B_D(\boldsymbol{k})$ fulfill a recursion relation . . .

$$B_{D+1}(\boldsymbol{k}) \;=\; B_1(\boldsymbol{k})\, B_D(\boldsymbol{k}) - D\, B_{D-1}(\boldsymbol{k}) \quad + \mathcal{O}(1/\sqrt{d})$$

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

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

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

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

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

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

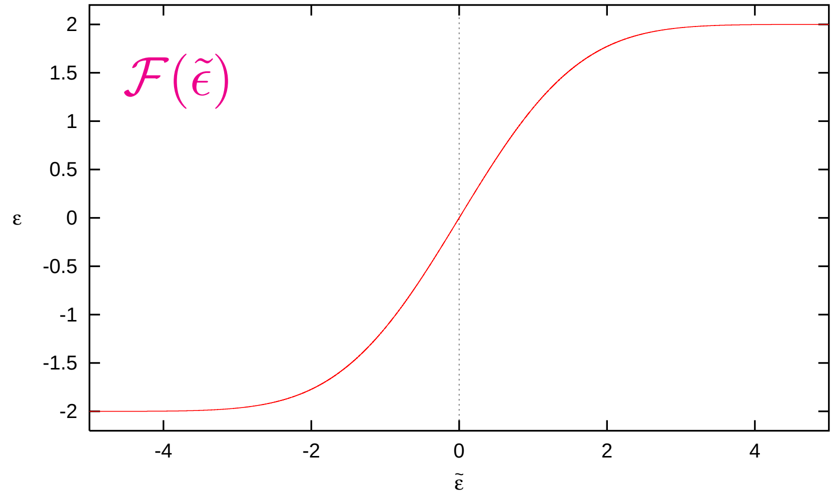
$$\mathcal{F}^{-1}(\epsilon) = \sqrt{2}\, \mathrm{erf}^{-1}\left(2 \int_{-\infty}^{\epsilon} \mathrm{d}\epsilon'\, \rho(\epsilon') - 1\right)$$

Redefinition of the Bethe Lattice

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

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

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



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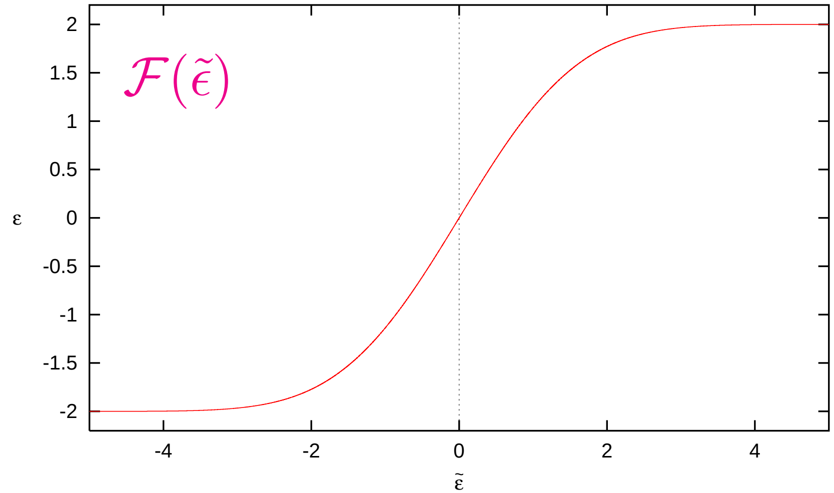

D	t^*_D	$\sum_{n=1}^{D} {t^*_n}^2$
1	0.98731	0.974773
3	-0.15353	0.998345
5	0.03893	0.999861
7	-0.01125	0.999987
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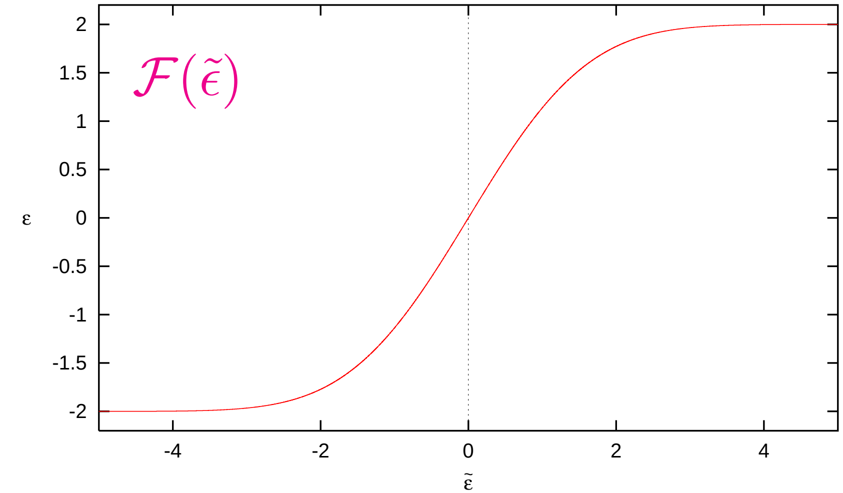

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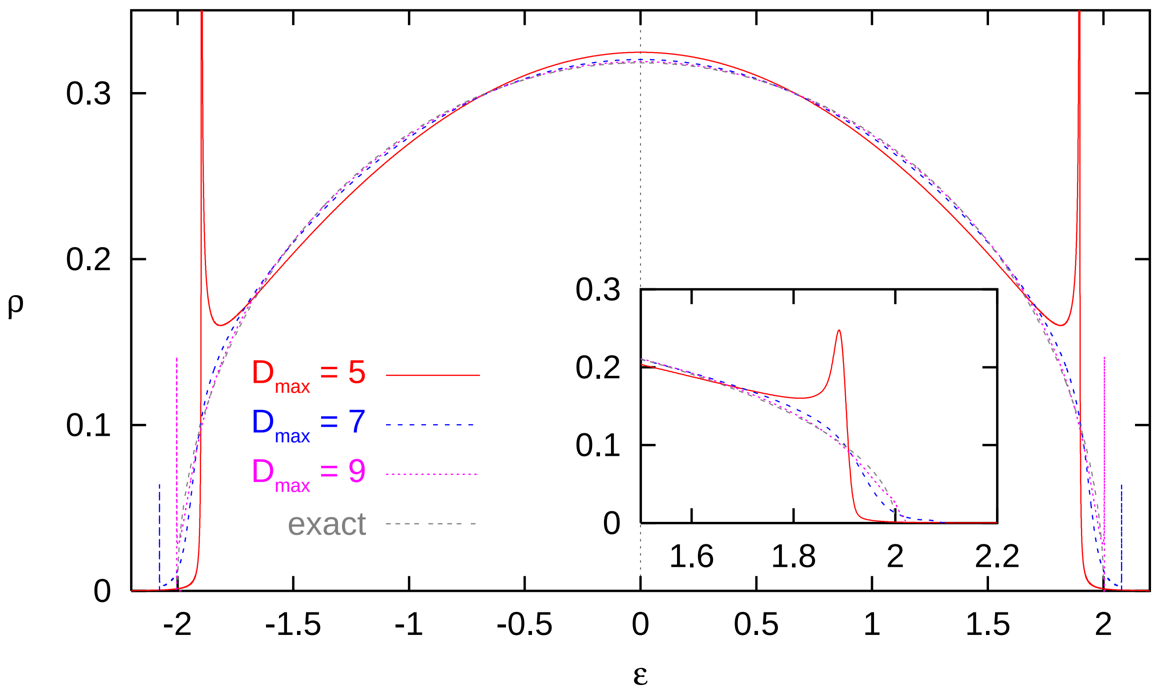
fast convergence with hopping cutoff $D_{\max}$



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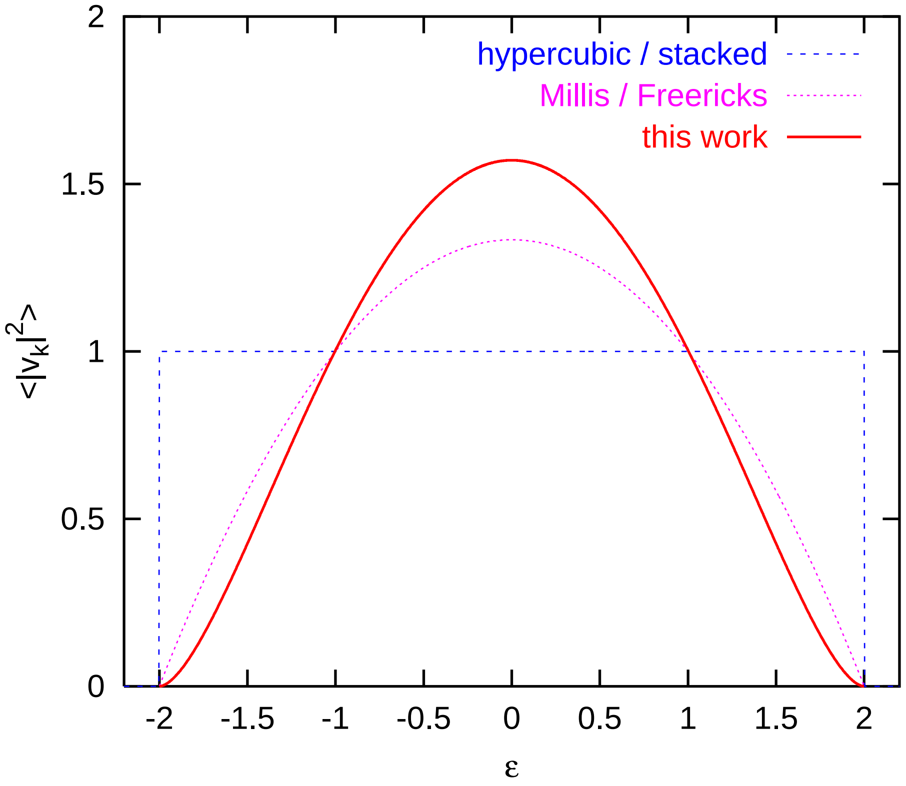
9	0.00343	0.999999

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

Specifically, for Bethe semi-elliptic DOS:

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



$\langle|\boldsymbol{v}_{\boldsymbol{k}}|^2\rangle \rightarrow 0$ at band edges

band center: max. transport contribution

other transport properties: analogous

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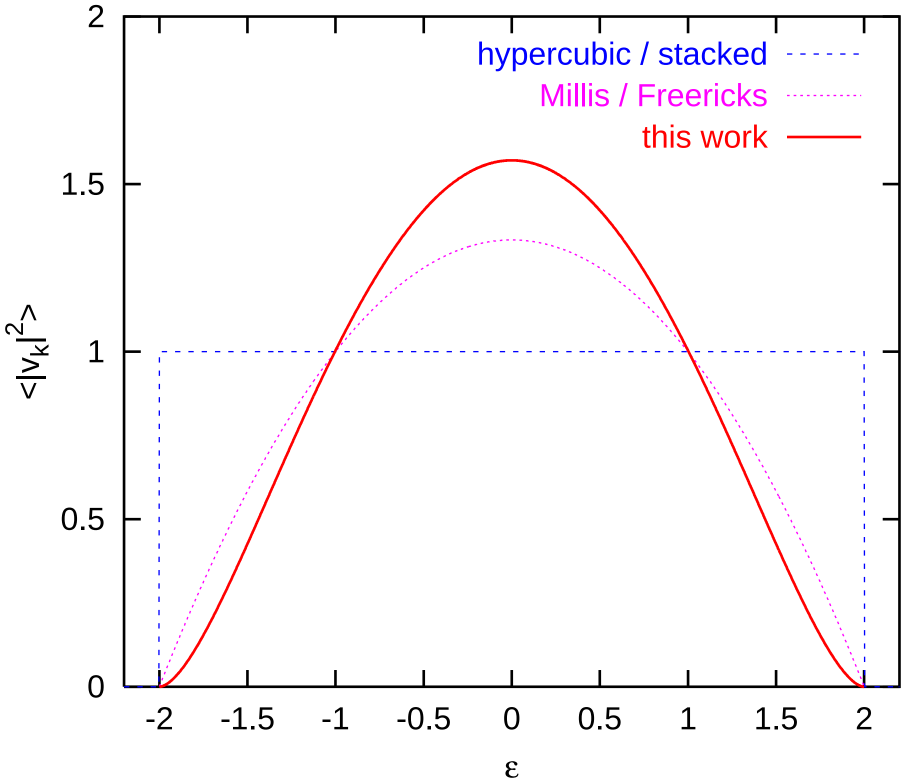

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f-sum: $\displaystyle\int_0^\infty \mathrm{d}\omega\,\sigma_{xx}(\omega) = \frac{\sigma_0}{4d}\left\langle\frac{\tilde\rho'(\epsilon)}{\rho(\epsilon)}\right\rangle = \frac{\sigma_0}{4d}\left\langle\left[\mathcal{F}''\big(\mathcal{F}^{-1}(\epsilon)\big)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

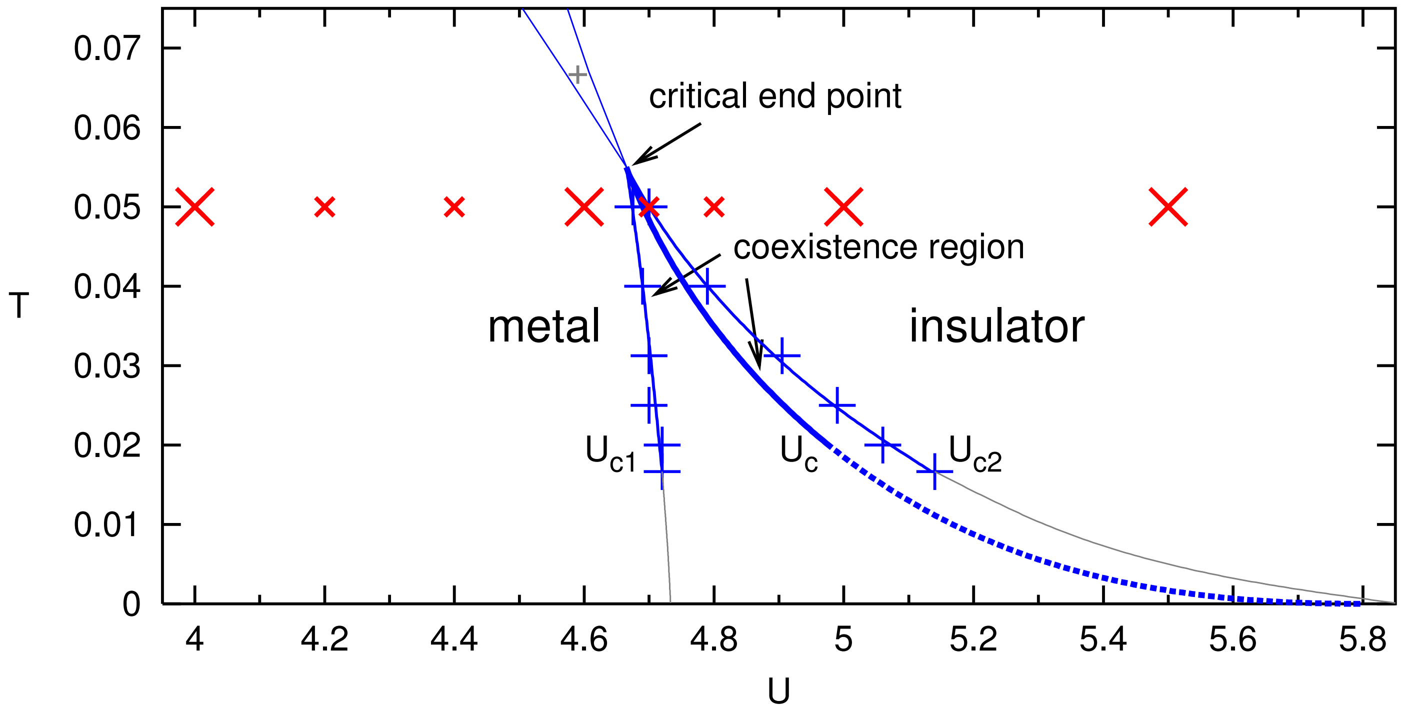
Numerical QMC/MEM Results for Half-filled Hubbard Model

For orientation:
MIT phase diagram

Bethe DOS, $W = 4$

results for $T = 0.05$

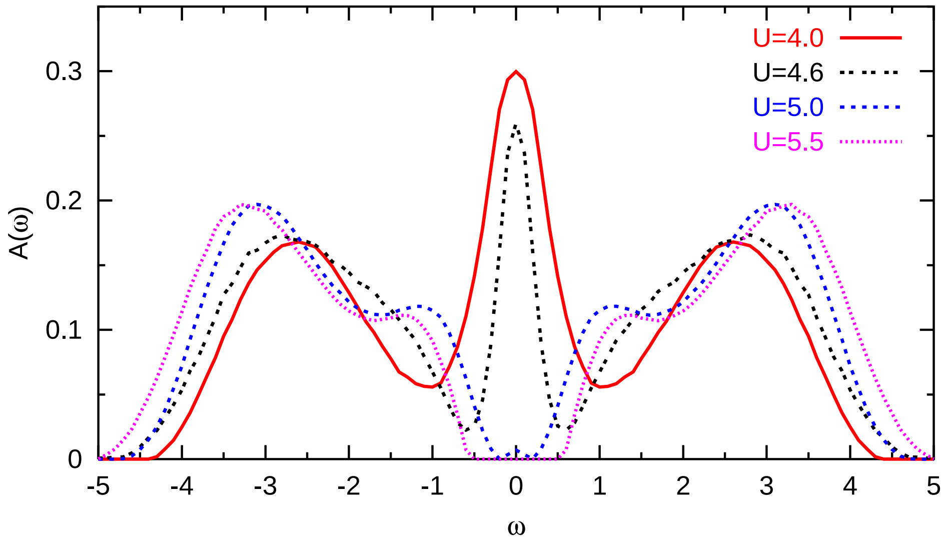
MIT at $U_c \approx 4.7$



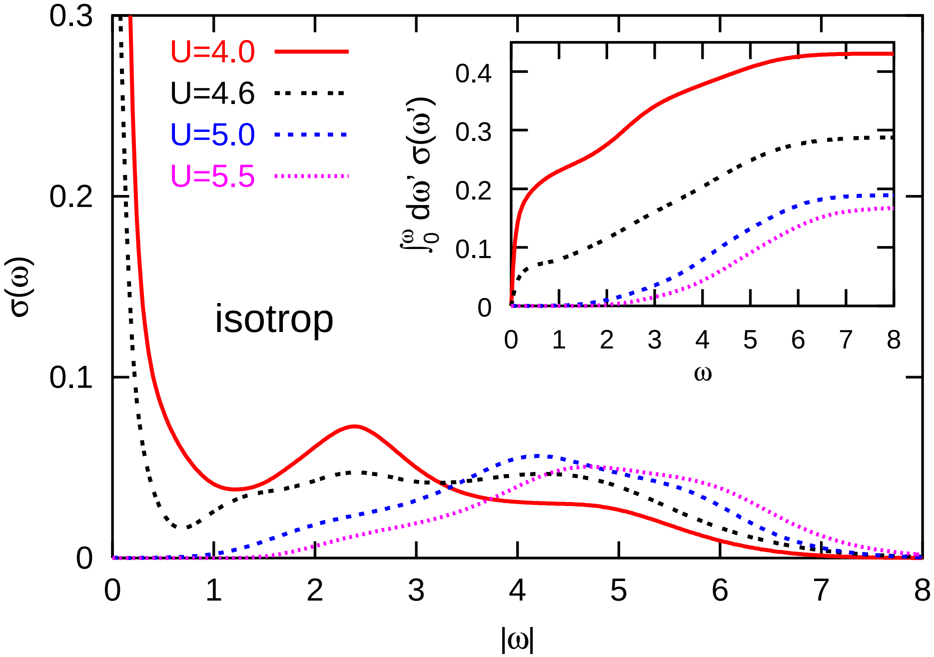
Quantum Monte-Carlo (QMC) with discretization $\Delta\tau = 0.1$

Analytical continuation using Maximum Entropy method

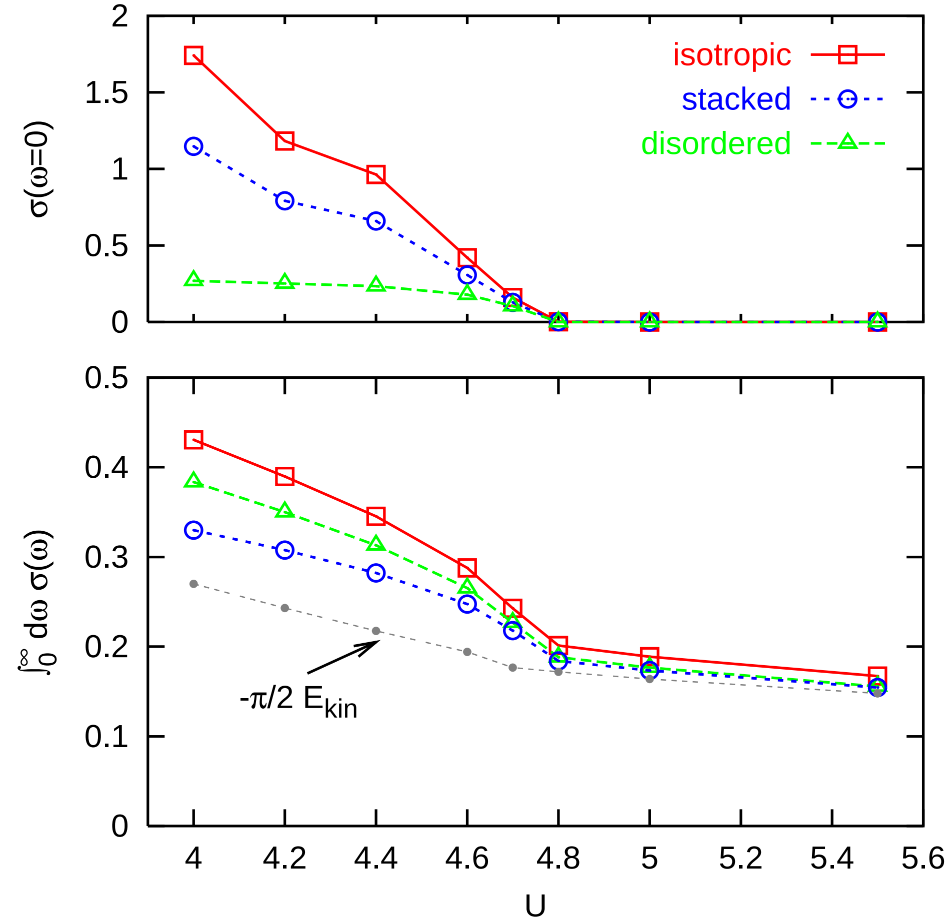
Local spectral function $A(\omega)$



Optical conductivity $\sigma(\omega)$



dc conductivity / f-sum



Conclusion

hc+NN DMFT transport formulae strongly modified for general lattices / hopping

e.g.: $t-t'$ model

construction method for lattice models (hc symmetry) with arbitrary DOS in large d

first Bravais lattice tb model with finite band edges in $d \to \infty$ and nonsingular $\mathbf{v_k}$

first definition of isotropic and coherent optical conductivity $\sigma(\omega)$ in high d consistent with Bethe semi-elliptic DOS

small impact of truncation (D_{max}) and of application in finite d

works as heuristic scheme in finite d (also multiple bands)

new DMFT f-sum rule

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

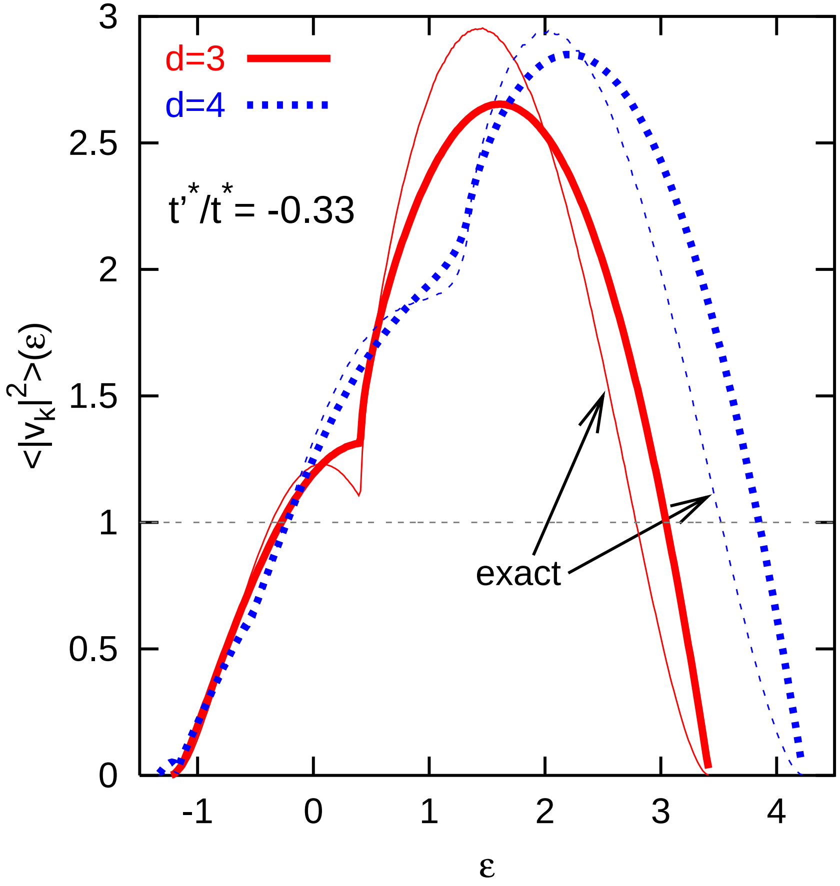
not discussed: vertex corrections, reduced umklapp scattering in finite d

http://www.physik.uni-augsburg.de/theo3/diss.de.shtml

http://komet337.physik.uni-mainz.de/Bluemer/talks.de.shtml

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