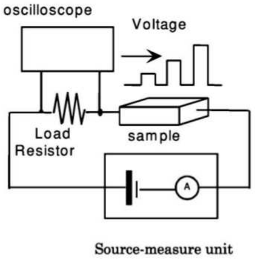
Correlated Electrons Driven by an Electric Field

C. Aron, G. Kotliar, C. Weber

Rutgers University



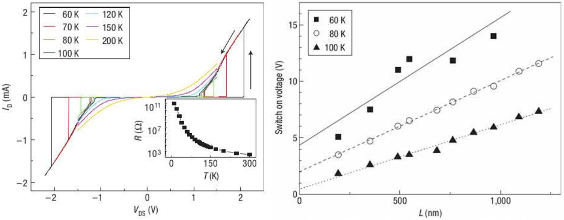
Phys. Rev. Lett. **108**, 086401 (2012)

+ arXiv:1203.3540 (2012)

Nonlinear transport of correlated electrons

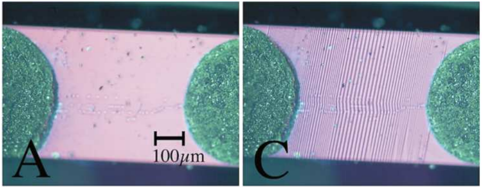
Ex: Magnetite (Fe_3O_4)

Group of Prof. Doug. Natelson @ Rice Nature Materials **7, 130 (2007)**

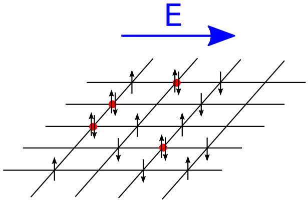


Ex: Organic molecular Mott insulator

Group of Prof. Y. Tokura @ Tsukuba Science **284, 1645 (1999)**



Correlated metal + Electric field



ex: 2d Hubbard model

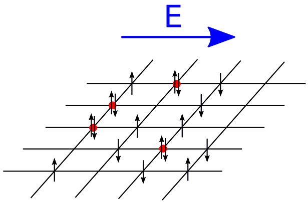
$$\mathcal{H}_s = -t \sum_{\langle ij\rangle\,\sigma} \left[c^\dagger_{i\sigma} \mathrm{e}^{\mathrm{i}\alpha_{ij}(t)} c_{j\sigma} + \mathrm{h.c.} \right] + \sum_{i\,\sigma=\uparrow,\downarrow} \phi_i(t) c^\dagger_{i\sigma} c_{i\sigma} + U \sum_i c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow}$$

$$\alpha_{ij}(t) \equiv q \int_{\mathbf{x}_j}^{\mathbf{x}_i} \mathrm{d}\mathbf{x} \cdot \mathbf{A}(t, \mathbf{x})$$

Gauges

Coulomb: $(\phi, \mathbf{A}) = (0, -\mathbf{E}t)$, Temporal: $(\phi, \mathbf{A}) = (-q\mathbf{E} \cdot \mathbf{x}, 0)$

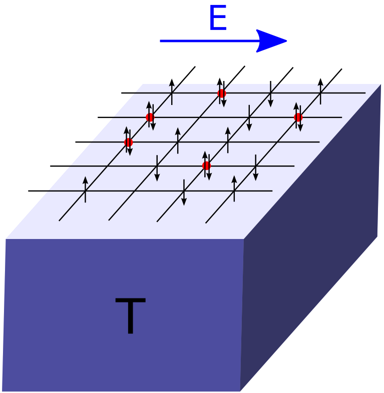
Correlated metal + Electric field

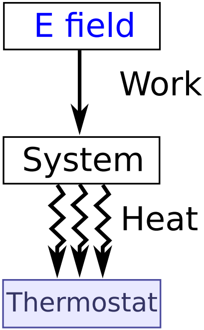


Steady states are impossible

- $U = 0 \Rightarrow$ Bloch oscillations
- $U \neq 0 \Rightarrow$ Current $\mathbf{J} \neq 0 \leftrightarrow$ Work $\mathcal{W} = \mathbf{J} \cdot \mathbf{E} > 0$

Correlated metal + Electric field + Dissipation





Coupling to a thermostat at temperature T

$$\mathcal{H}_{sb} = V \sum_{i\sigma l} \mathrm{e}^{\mathrm{i}\theta_i(t)} b^\dagger_{i\sigma l} c_{i\sigma} + \mathrm{h.c.}$$

$$\theta_i(t) \equiv \int^t \mathrm{d}t' \, \phi_i(t')$$

Effect of dissipation on the Mott physics

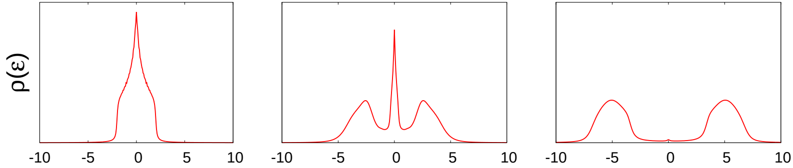
Local density of states $\rho(\epsilon)$

$U = 0$ **Metal** $\Longleftarrow$

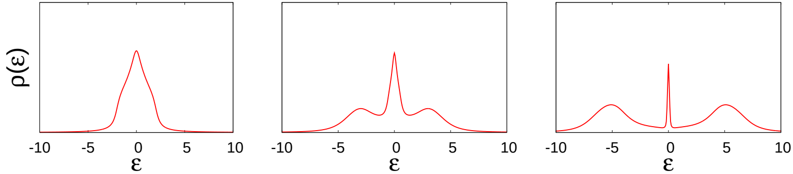
$U = 5$

$U = 10$ $\Longrightarrow$ **Insulator**

$\Gamma = 0.05$



$\Gamma = 0.30$



Real-time dynamics

Schwinger-Keldysh formalism

$$\mathbf{G} = \begin{pmatrix} G^K & G^R \\ \check{G}^R & 0 \end{pmatrix} \quad \mathbf{\Sigma} = \begin{pmatrix} 0 & \check{\Sigma}^R \\ \Sigma^R & \Sigma^K \end{pmatrix}$$

Schwinger-Dyson equation(s)

$$\mathbf{G}(t,\mathbf{x};t',\mathbf{x}') = \mathbf{G_0}(t,\mathbf{x};t',\mathbf{x}') + \mathbf{G_0} \circ \mathbf{\Sigma} \circ \mathbf{G}(t,\mathbf{x};t',\mathbf{x}')$$

Steady-state solutions

Space & time translational invariance

Real-time dynamics

Schwinger-Keldysh formalism

$$\mathbf{G} = \begin{pmatrix} G^K & G^R \\ \check{G}^R & 0 \end{pmatrix} \quad \mathbf{\Sigma} = \begin{pmatrix} 0 & \check{\Sigma}^R \\ \Sigma^R & \Sigma^K \end{pmatrix}$$

Schwinger-Dyson equation(s)

$$\mathbf{G}(t,\mathbf{x};t',\mathbf{x}') = \mathbf{G_0}(t,\mathbf{x};t',\mathbf{x}') + \mathbf{G_0} \circ \mathbf{\Sigma} \circ \mathbf{G}(t,\mathbf{x};t',\mathbf{x}')$$

Steady-state solutions

Space & time translational invariance
is broken (artificially) by every choice of gauge !

$\Rightarrow$ Need for a gauge invariant formalism

Gauge invariant formalism

Wigner transform

$$\mathbf{G}\begin{pmatrix} t, & \mathbf{x} \\ t', & \mathbf{x}' \end{pmatrix} \overset{chg.var.}{\longmapsto} \mathbf{G}\begin{pmatrix} T \equiv \frac{t+t'}{2}, & \mathbf{X} \equiv \frac{\mathbf{x}+\mathbf{x}'}{2} \\ \bar{t} \equiv t - t', & \bar{\mathbf{x}} \equiv \mathbf{x} - \mathbf{x}' \end{pmatrix} \overset{\mathcal{FT}}{\longmapsto} \mathbf{G}(T, \mathbf{X}; \omega, \mathbf{k})$$

Gauge invariant formalism

Wigner transform

$$\mathbf{G}\begin{pmatrix} t, & \mathbf{x} \\ t', & \mathbf{x}' \end{pmatrix} \overset{chg.var.}{\longmapsto} \mathbf{G}\begin{pmatrix} T \equiv \frac{t+t'}{2}, & \mathbf{X} \equiv \frac{\mathbf{x}+\mathbf{x}'}{2} \\ \bar{t} \equiv t - t', & \bar{\mathbf{x}} \equiv \mathbf{x} - \mathbf{x}' \end{pmatrix} \overset{\mathcal{FT}}{\longmapsto} \mathbf{G}(T, \mathbf{X}; \omega, \mathbf{k})$$

Change of variables

$$\begin{aligned} \omega &\mapsto \quad \omega - \phi(T, \mathbf{X}) \equiv \varpi \\ \mathbf{k} &\mapsto \quad \mathbf{k} - q\mathbf{A}(T, \mathbf{X}) \equiv \boldsymbol{\kappa} \end{aligned} \implies \text{Gauge invariant } \mathbf{G}(T, \mathbf{X}; \varpi, \boldsymbol{\kappa})$$

Gauge invariant formalism

Wigner transform

$$\mathbf{G}\begin{pmatrix} t, & \mathbf{x} \\ t', & \mathbf{x}' \end{pmatrix} \overset{chg.var.}{\longmapsto} \mathbf{G}\begin{pmatrix} T \equiv \frac{t+t'}{2}, & \mathbf{X} \equiv \frac{\mathbf{x}+\mathbf{x}'}{2} \\ \overline{t} \equiv t - t', & \overline{\mathbf{x}} \equiv \mathbf{x} - \mathbf{x}' \end{pmatrix} \overset{\mathcal{FT}}{\longmapsto} \mathbf{G}(T, \mathbf{X}; \omega, \mathbf{k})$$

Change of variables

$$\begin{aligned} \omega &\mapsto \omega - \phi(T, \mathbf{X}) \equiv \varpi \\ \mathbf{k} &\mapsto \mathbf{k} - q\mathbf{A}(T, \mathbf{X}) \equiv \boldsymbol{\kappa} \end{aligned} \implies \text{Gauge invariant } \mathbf{G}(T, \mathbf{X}; \varpi, \boldsymbol{\kappa})$$

Space & time translational invariance: $\cancel{T}, \cancel{\mathbf{X}} \implies \mathbf{G}(\varpi, \boldsymbol{\kappa})$

Gauge invariant formalism

Wigner transform

$$\mathbf{G}\begin{pmatrix} t, & \mathbf{x} \\ t', & \mathbf{x}' \end{pmatrix} \overset{chg.var.}{\longmapsto} \mathbf{G}\begin{pmatrix} T \equiv \frac{t+t'}{2}, & \mathbf{X} \equiv \frac{\mathbf{x}+\mathbf{x}'}{2} \\ \bar{t} \equiv t - t', & \bar{\mathbf{x}} \equiv \mathbf{x} - \mathbf{x}' \end{pmatrix} \overset{\mathcal{FT}}{\longmapsto} \mathbf{G}(T, \mathbf{X}; \omega, \mathbf{k})$$

Change of variables

$$\begin{aligned} \omega &\mapsto \omega - \phi(T, \mathbf{X}) \equiv \varpi \\ \mathbf{k} &\mapsto \mathbf{k} - q\mathbf{A}(T, \mathbf{X}) \equiv \boldsymbol{\kappa} \end{aligned} \implies \text{Gauge invariant } \mathbf{G}(T, \mathbf{X}; \varpi, \boldsymbol{\kappa})$$

Space & time translational invariance: $\cancel{T}, \cancel{\mathbf{X}} \implies \mathbf{G}(\varpi, \boldsymbol{\kappa})$

Steady-state Schwinger-Dyson equations

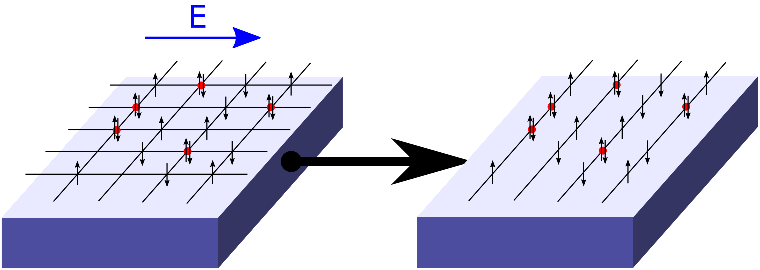
$$\begin{aligned} \mathbf{G}(\varpi, \boldsymbol{\kappa}) &= \mathbf{G_0}(\varpi, \boldsymbol{\kappa}) + \mathbf{G_0} \star \boldsymbol{\Sigma} \star \mathbf{G}(\varpi, \boldsymbol{\kappa}) \\ \star &\equiv \exp\left(\tfrac{i}{2} q [\overleftarrow{\partial_\varpi} \overrightarrow{\mathbf{E} \cdot \nabla_{\boldsymbol{\kappa}}} - \overleftarrow{\mathbf{E} \cdot \nabla_{\boldsymbol{\kappa}}} \overrightarrow{\partial_\varpi}]\right) \end{aligned}$$

Dimensional reduction

In the $E \to \infty$ limit,

the out-of-equilibrium d-dimensional system reduces to an *equilibrium* system in the $d-1$ dimensions perpendicular to the field.

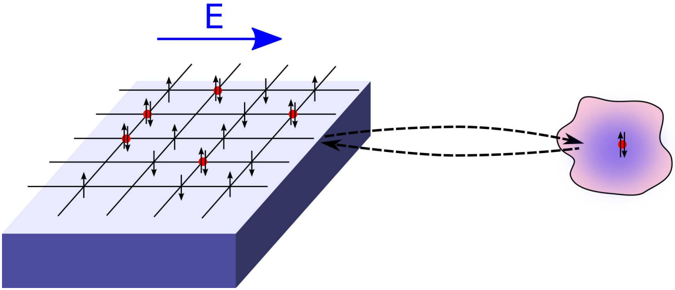
$$\mathbf{G}(\varpi, \boldsymbol{\kappa}_\perp) = \mathbf{G_0}(\varpi, \boldsymbol{\kappa}_\perp) + \mathbf{G_0}\,\boldsymbol{\Sigma}\,\mathbf{G}(\varpi, \boldsymbol{\kappa}_\perp)$$



Phys. Rev. Lett. **108**, 086401 (2012)

Dynamical Mean-Field Theory

$$\mathbf{\Sigma}_\mathbf{U}[\mathbf{G}(\varpi,\boldsymbol{\kappa})] \simeq \mathbf{\Sigma}_\mathbf{U}^{\mathbf{imp}}[\mathcal{G}(\varpi)]$$



Dynamical Mean-Field Theory

1 – Build the impurity problem

$$\text{Impurity}\left\{\begin{array}{ll}\mathcal{G}^R(\varpi) = & \left[G^R_{loc}(\varpi)^{-1} + \Sigma^R_U(\varpi)\right]^{-1} \\ \mathcal{G}^K(\varpi) = & \left|\mathcal{G}^R(\varpi)\right|^2 \left[\frac{G^K_{loc}(\varpi)}{\left|G^R_{loc}(\varpi)\right|^2} - \Sigma^K_U(\varpi)\right]\end{array}\right\}\text{Lattice}$$

$$G_{loc}(\varpi) \equiv \int \mathrm{d}\boldsymbol{\kappa}\; G(\varpi, \boldsymbol{\kappa}) / \int \mathrm{d}\boldsymbol{\kappa}$$

2 – Solve the impurity problem

$$\boldsymbol{\Sigma}^{\mathbf{imp}}_{\mathbf{U}}[\mathcal{G}] \simeq U^2 \text{ “ } \mathcal{G}^3 \text{ ”}$$

3 – Mean-Field approximation

$$\boldsymbol{\Sigma}_{\mathbf{U}}(\varpi, \boldsymbol{\kappa}) \simeq \boldsymbol{\Sigma}^{\mathbf{imp}}_{\mathbf{U}}[\mathcal{G}(\varpi)]$$

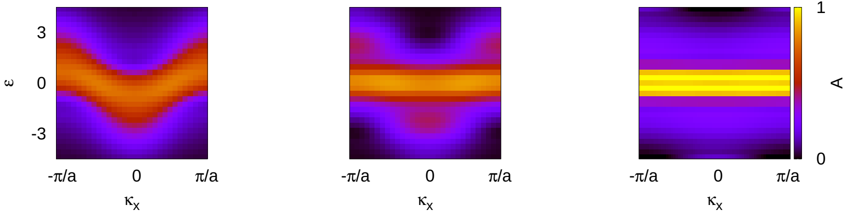
4 – Solve the lattice problem

$$\mathbf{G}(\varpi, \boldsymbol{\kappa}) = \mathbf{G_0}(\varpi, \boldsymbol{\kappa}) + \mathbf{G_0} \star \boldsymbol{\Sigma} \star \mathbf{G}(\varpi, \boldsymbol{\kappa})$$

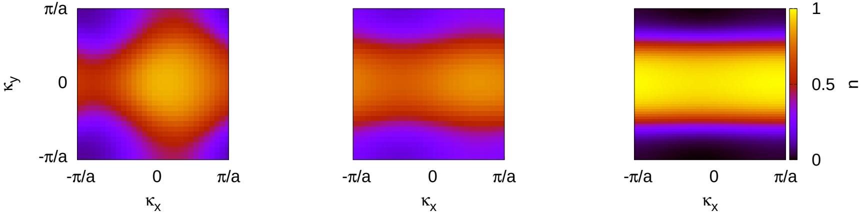
Dimensional crossover of the metal

Spectral function $A(\epsilon, \boldsymbol{\kappa}) = -\text{Im } G^R(\epsilon, \boldsymbol{\kappa})/\pi$

$E = 1$ $E = 5$ $E = 10$



Momentum distribution function $n(\boldsymbol{\kappa})$

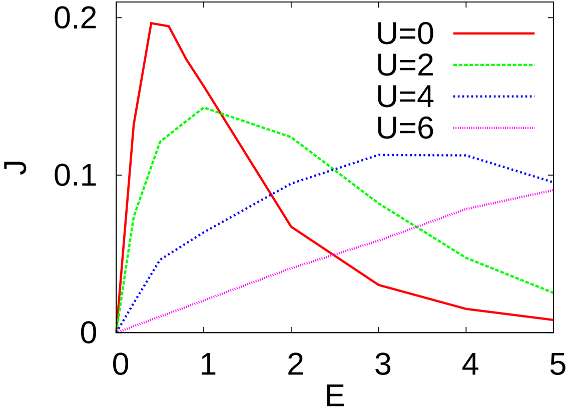


$U = 3$

half filling

Dimensional crossover of the metal

Current density **J**(**E**)

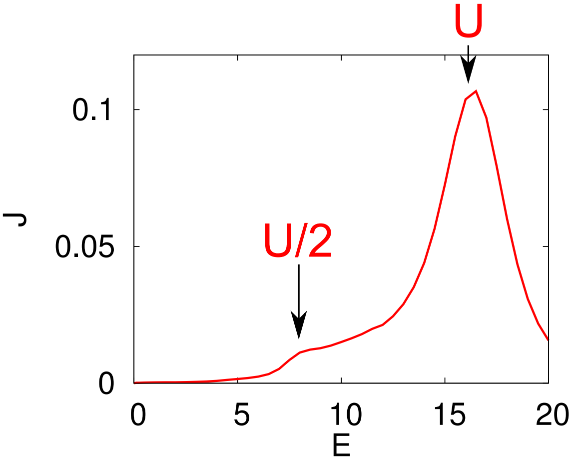


half-filling

Phys. Rev. Lett. **108**, 086401 (2012)

Dielectric breakdown of the Mott insulator

Current density $\mathbf{J}(E)$



$U = 16$, $\Gamma = 0.20$
half-filling

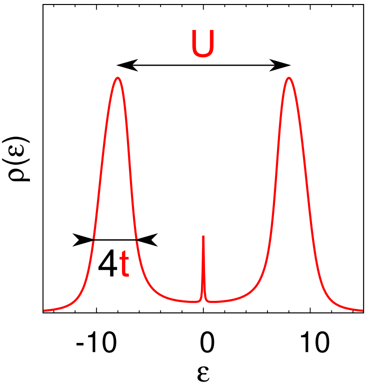
arXiv:1203.3540 (2012)

Dimensional crossover of the Mott insulator

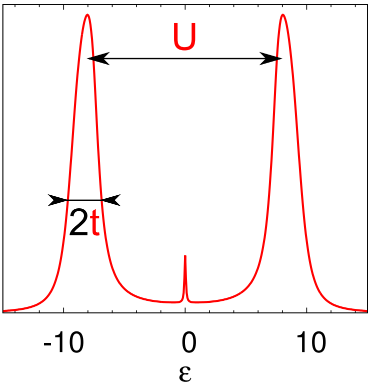
Local density of states $\rho(\epsilon)$

$E = 0$ $\Longrightarrow$ $E \mapsto \infty$

$2d$



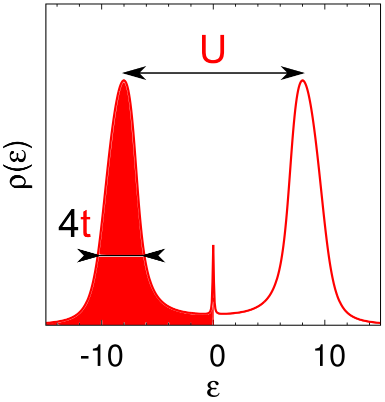
$1d$

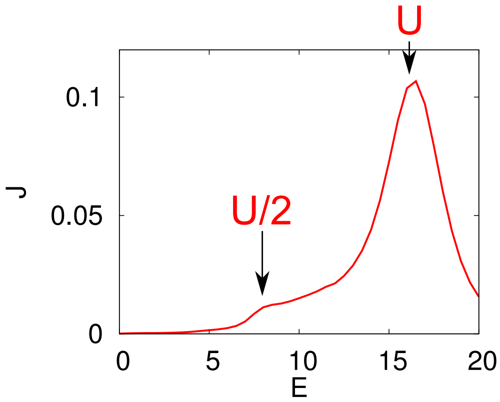


$U = 16$, $\Gamma = 0.20$

half-filling

Dielectric breakdown of the Mott insulator



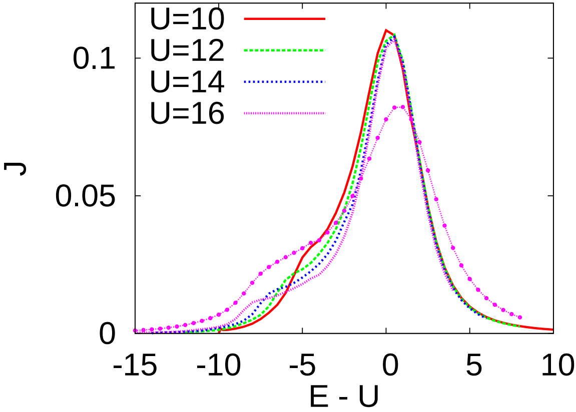


$U = 16$, $\Gamma = 0.20$,
half-filling

Dielectric breakdown of the Mott insulator

Current

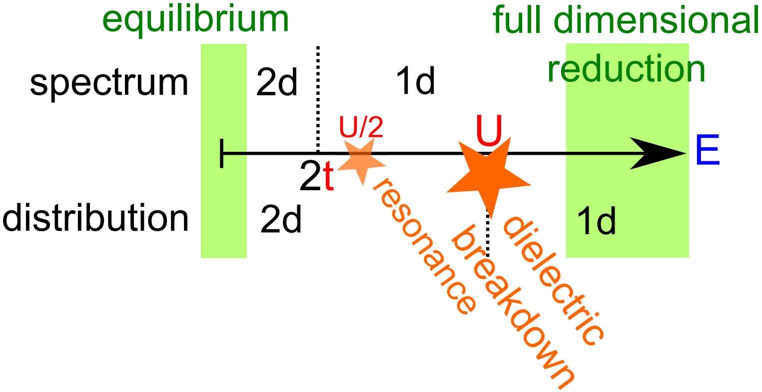
J(**E**)



Γ = 0.20 and 0.35

Fate of the electric field driven Mott insulator

Spectral properties and distribution functions crossover to 1*d* at different energy scales.



Electric field driven correlated electrons – Summary

- Physical setup: need for a dissipation mechanism, Γ
- Theoretical approach: gauge invariant formalism
- Generic result: dimensional reduction for $E \mapsto \infty$
- Technique at finite U & E: DMFT directly in the NESS
- Out-of-equilibrium phase diagram:
  - illustration of the dimensional crossover
  - non-linear transport properties
  - dielectric breakdown of the Mott insulator

Star product

$$\star \equiv \exp\left(\frac{\mathrm{i}}{2} q [\overleftarrow{\partial_\varpi} \overrightarrow{\mathbf{E}\cdot\boldsymbol{\nabla}_{\boldsymbol{\kappa}}} - \overleftarrow{\mathbf{E}\cdot\boldsymbol{\nabla}_{\boldsymbol{\kappa}}} \overrightarrow{\partial_\varpi}]\right)$$

Compute $[f \star g](\varpi, \boldsymbol{\kappa})$

$$\underbrace{\begin{array}{ccc} f(\varpi,\boldsymbol{\kappa}) & & g(\varpi,\boldsymbol{\kappa}) \\ \downarrow \mathcal{FT}^{-1} & & \mathcal{FT}^{-1}\downarrow \\ f(\tau;\boldsymbol{\kappa}) & & g(\tau;\boldsymbol{\kappa}) \end{array}}$$

$$\downarrow$$

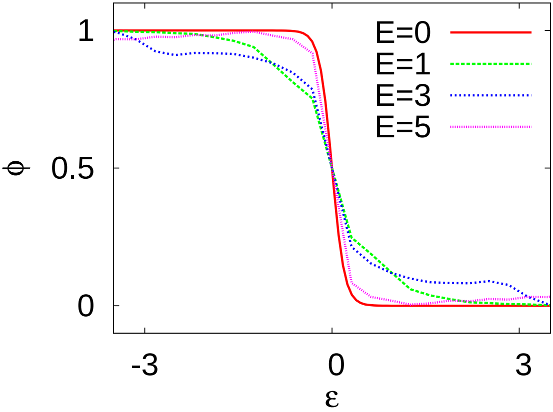
$$[f \star g](\tau;\boldsymbol{\kappa}) = \int \mathrm{d}\tau'\, f\left(\tau - \tau'; \boldsymbol{\kappa} + q\mathbf{E}\frac{\tau'}{2}\right) g\left(\tau'; \boldsymbol{\kappa} + q\mathbf{E}\frac{\tau'-\tau}{2}\right)$$

$$\downarrow \mathcal{FT}$$

$$[f \star g](\varpi, \boldsymbol{\kappa})$$

Dimensional Crossover

Distribution function $\phi(\epsilon) = \left[1 + G^K_{loc}(\epsilon)/\text{Im } G^R_{loc}(\epsilon)\right]/2$



U=3, energies in units of $2t$, $a = q = 1$