Real Time Green's Functions from NCA based Impurity Solver

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Introduction

Strongly correlated materials.

- Idea of description of electrons in solids as independent particles
  $\rightarrow$ wave-like picture
- Materials in which electrons tend to *localize*
  $\rightarrow$particle-like picture
- Strong electronic correlations brings out a variety of phenomena, e.g. metal-to-Mott-insulator transitions

Description of the lattice

Hubbard model.

$$H_{\mathrm{Hubbard}} = -\sum_{\langle i,j\rangle,\sigma} t_{ij} d^{\dagger}_{i\sigma} d_{j\sigma} + \sum_{i} U\left(d^{\dagger}_{i\uparrow} d_{i\uparrow} - \frac{1}{2}\right)\left(d^{\dagger}_{i\downarrow} d_{i\downarrow} - \frac{1}{2}\right)$$

- $t_{ij} \simeq$ overlap between orbitals on neighbouring atomic sites $\sim \mathrm{eV}$
- Coulomb repulsion U, screened value $\sim \mathrm{eV}$

$\rightarrow$ competition between energy scales

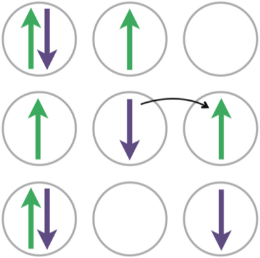

Figure 1: Lattice model

source: H. Aoki, N. Tsuji, M. Eckstein, M. Kollar, T. Oka, and P. Werner, Rev. Mod. Phys. 86, 779 (2014)

Dynamical Mean Field Theory

Idea of mapping.

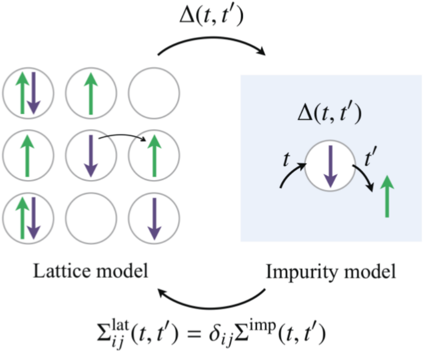

Figure 2: Mapping of the lattice problem onto an Impurity problem

- Approximate lattice problem with many degrees of freedom by *single-site problem*

Dynamical Mean Field Theory

Set of self-consistent equations.

- compute local Greens function $G^{\sigma}_{ii}(t-t') = -i\langle \mathscr{T} d_{i\sigma}(t) d^{\dagger}_{i\sigma}(t')\rangle$ from an effective impurity model with action

$$S = i\int_c dt U n_\uparrow(t) n_\downarrow(t) - i\sum_\sigma \int_c dt dt' d^\dagger_\sigma(t) \triangle(t-t') d_\sigma(t').$$

- use impurity self energy, defined via $G^{-1}_{ii}(\omega) = \omega + \mu - \triangle(\omega) - \Sigma^{imp}(\omega)$, to obtain the lattice Greens function

$$G^{-1}_{ij}(\omega) = \delta_{ij}[\omega + \mu - \Sigma_{ii}(\omega)] - v_{ij}$$

$$\Sigma_{ii}(\omega) \simeq \Sigma^{imp}(\omega); \Sigma_{i\neq j}(\omega) \simeq 0$$

- average over the Brillouin zone to get the on-site component:

$$G_{ii}(\omega) = \frac{1}{L}\sum_k G_k(\omega) = \frac{1}{L}\sum_k \frac{1}{\omega + \mu + \Sigma(\omega) - \varepsilon_k}$$

Dynamical Mean Field Theory

Set of self-consistent equations.

$$\mathscr{G}_0 = \omega + \mu - \triangle(\omega)$$

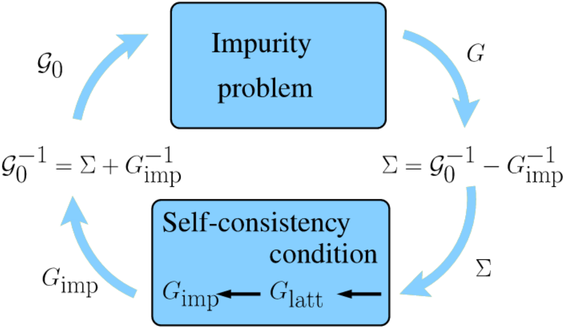

Figure 3: DMFT iterative loop

source: B. Amadon, Journal of Physics: Condensed Matter, Volume 24, Number 7

Real Time Impurity Solver

Pertubative expansion.

Single-orbital Anderson impurity model

$$\mathrm{H_{imp}} = \mathrm{H_{loc}} + \mathrm{H_{bath}} + \mathrm{H_{hyb}}$$

$$\mathrm{H_{loc}} = \sum_{\sigma \in \uparrow,\downarrow} \varepsilon_\sigma \mathrm{d}^\dagger_\sigma \mathrm{d}_\sigma + \mathrm{U}(\mathrm{n}_\uparrow - \mu)(\mathrm{n}_\downarrow - \mu)$$

$$\mathrm{H_{bath}} = \sum_{\sigma,\lambda} \varepsilon_\lambda \mathrm{b}^\dagger_\lambda \mathrm{b}_\lambda$$

$$\mathrm{H_{hyb}} = \sum_{\sigma,\lambda} (\mathrm{v}_{\sigma\lambda} \mathrm{b}^\dagger_\lambda \mathrm{d}_\sigma + \mathrm{v}^*_{\sigma\lambda} \mathrm{d}^\dagger_\sigma \mathrm{b}_\lambda)$$

- Write impurity Hamiltonian as a sum $\mathrm{H_{imp}} = \mathrm{H_0} + \mathrm{H_{int}}$
- Exact time evolution for H_0, pertubative expansion for $\mathrm{H_{int}}$

Real Time Impurity Solver

Calculation of expectation values.

- Goal is to evaluate objects like $G^{<}(t,t') = i\langle d^{\dagger}(t')d(t)\rangle$ and $G^{>}(t,t') = -i\langle d(t)d^{\dagger}(t')\rangle$
- Expectation values are given by $\langle O(t)\rangle = \mathrm{Tr}\left(\rho U^{\dagger}(t)\hat{O}U(t)\right)$
- Interaction picture propagator $U(t) = \exp^{iH_0 t}\exp^{-iHt}$ and operator $\hat{O}(t) = \exp^{iH_0 t} O \exp^{-iH_0 t}$
- Reduced Hamiltonian $H_0 = H_{imp} - H_{hyb}$

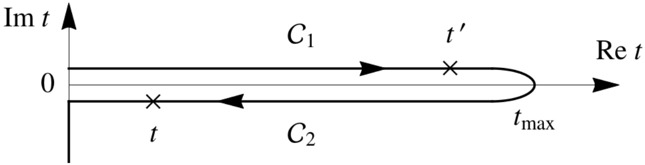

Figure 4: Keldysh Contour

source: H. Aoki, N. Tsuji, M. Eckstein, M. Kollar, T. Oka, and P. Werner, Rev. Mod. Phys. 86, 779 (2014)

Real Time Impurity Solver

Hybridization expansion.

- Expansion of U(t) and $U^{\dagger}(t)$ in terms of $\widehat{H}_{hyb}$:

$$U(t) = \sum_{n=0}^{\infty} (-i)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n \widehat{H}_{hyb}(t_1)\widehat{H}_{hyb}(t_2) \cdots \widehat{H}_{hyb}(t_n)$$

- Insert expansion for U(t) into propagator between many body states:

$$G_{\alpha\beta}(t) = \langle\langle \alpha \mid \rho_D \exp^{-iHt} \mid \beta \rangle\rangle_B = \langle\langle \alpha \mid \rho_D \exp^{-iH_0 t} U(t) \mid \beta \rangle\rangle_B$$

- many body states are $|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle$
- $\langle \cdots \rangle_B = \mathrm{Tr}\{\rho_B \cdots\}$

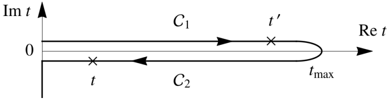

Figure 5: Keldysh Contour

Real Time Impurity Solver

Hybridization expansion.

$$G_{\alpha\alpha}(t) = G^{(0)}_{\alpha\alpha}(t) - \sum_{\gamma\delta}\int_0^t dt_1 \int_0^{t_1} dt_2 G^{(0)}_{\alpha\alpha}(t-t_1) G^{(0)}_{\beta\beta}(t_1-t_2) \triangle^{\gamma\delta}_{\alpha\beta}(t_1-t_2) G^0_{\alpha\alpha}(t_2) - \cdots$$

with bare propagators

$$G^{(0)}_{\alpha\alpha}(t) = \langle\langle \alpha \mid \rho_D \exp^{-iH_0 t} \mid \alpha\rangle\rangle_B = \exp^{-i\varepsilon_\alpha t}$$

and Hybridization

$$\begin{aligned}\triangle_{\alpha\beta}(t_1-t_2) = {} & \langle \alpha \mid d_\sigma \mid \beta\rangle\langle\beta \mid d^\dagger_\sigma \mid \alpha\rangle \triangle^{<}(t_1-t_2) + \\ & \langle \alpha \mid d^\dagger_\sigma \mid \beta\rangle\langle\beta \mid d_\sigma \mid \alpha\rangle \triangle^{>}(t_1-t_2)\end{aligned}$$

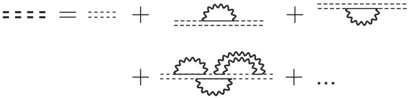

Figure 6: Example of diagrammatic expansion for bold propagators

Real Time Impurity Solver

Hybridization expansion.

Dyson equation

$$G_{\alpha\alpha}(t) = G^{(0)}_{\alpha\alpha}(t) + \int_0^t dt_1 \int_0^{t_1} dt_2 G^{(0)}_{\alpha\alpha}(t-t_1)\Sigma_{\alpha\alpha}(t_1-t_2)G_{\alpha\alpha}(t_2)$$

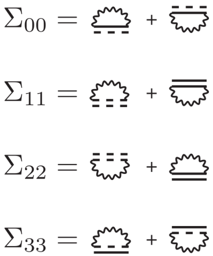

Figure 7: NCA Self-energy

Self-consistent solution

1. Initialize $G_{\alpha\alpha}(t)$ with $G^{(0)}_{\alpha\alpha}(t)$
2. Compute self-energy $\Sigma_{\alpha\alpha}(t)$
3. Update $G_{\alpha\alpha}(t)$
4. go back to step 2

source: G. Cohen, D. R. Reichman, A. J. M. and E. Gull; Phys. Rev. B89, 112139(2014)

Real Time Impurity Solver

Hybridization expansion.

Vertex functions

$$K_{\alpha\beta}(t,t') = K^{(0)}_{\alpha\beta}(t,t') + \sum_{\gamma\delta} \int_0^t dt_1 \int_0^{t'} dt_2 K_{\alpha\gamma}(t_1,t_2) \triangle_{\gamma\delta}(t_1,t_2) G^{\dagger}_{\delta\beta}(t-t_1) G_{\delta\beta}(t'-t_2).$$

$$K^{(0)}_{\alpha\beta}(t,t') = G^{\dagger}_{\alpha\beta}(t) G_{\alpha\beta}(t')$$

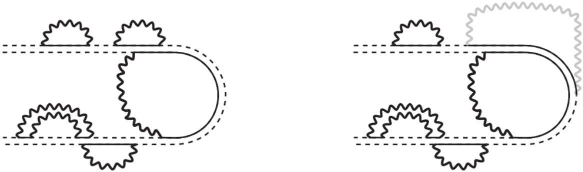

Figure 8: Diagrammatic expansion for Vertex functions

source: G. Cohen, D. R. Reichman, A. J. M. and E. Gull; Phys. Rev. B89, 112139(2014)

System

Bethe lattice in the initial Néel state.

Self-consistency condition

$$\Delta_{A(B),\sigma}(t,t') = v(t) G_{B(A),\sigma}(t,t') v^*(t')$$

Time-dependent electric field

$$\mathrm{H_{drv}(t) = \sum_j eaE_0 sin(\omega t) s_j n_j}$$

$$\mathrm{v_{ij}(t) = v_{ij}} \exp^{\mathrm{iA(s_i - s_j)cos(\omega t)}}$$

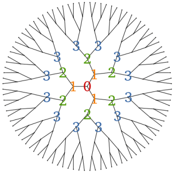

Figure 9: Structure of the Bethe lattice

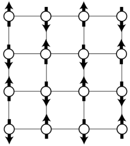

Figure 10: Classical anti-ferromagnetical Néel-state

Open systems

Free-fermion bath

$$\mathrm{H_{tot}} = \mathrm{H_{imp}} + \mathrm{H_{fBath}} + \mathrm{H_{fmix}}$$

$$\mathrm{H_{fBath}} = \sum_{\mathrm{k},\sigma} \varepsilon_{\mathrm{k}} \mathrm{f}^{\dagger}_{\mathrm{k},\sigma} \mathrm{f}_{\mathrm{k},\sigma}$$

$$\mathrm{H_{fmix}} = \sum_{\mathrm{k},\sigma} (\mathrm{V_k} \mathrm{f}^{\dagger}_{\mathrm{k},\sigma} \mathrm{d}_{\sigma} + \mathrm{V}^{*}_{\mathrm{k}} \mathrm{d}^{\dagger}_{\sigma} \mathrm{f}_{\mathrm{k},\sigma})$$

$$G(t,t') = (G_0^{-1}(t,t') - \Sigma_{fBath}(t,t') - \Sigma(t,t'))^{-1}$$

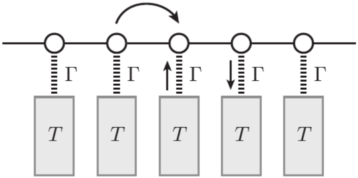

Figure 11: Schematic representation of a free-fermion bath model

Results

How does the ability to dissipate energy change in a non-equilibrium state?

$$I_E(t) = \langle \mathscr{I}_E(t) \rangle \text{ with } \mathscr{I}_E = \dot{H}_{fBath} = i\sum_{k,\sigma} \varepsilon_k (V_k d_\sigma f^\dagger_{k,\sigma} - V^*_k f_{k,\sigma} d^\dagger_\sigma)$$

$$P_{\omega_{probe}}(A_{probe}) = \lim_{A_{probe}\to 0} \frac{dI_E(A_{probe}(\omega_{probe}))}{dA_{probe}(\omega_{probe})} \simeq \frac{I_E(\Delta A_{probe}(\omega_{probe}))}{\Delta A_{probe}(\omega_{probe})}$$

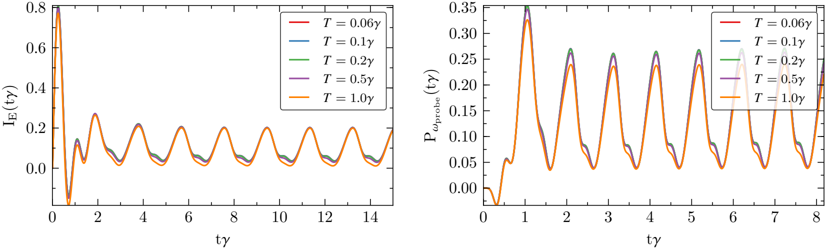

Figure 12: Example of heat current (left) and response (right) at resonant driving for a pump amplitude $A = 1.0$ and a probe filed with parameters $\omega_{probe} = 5$ and $A_{probe} = 0.1$.

Results

Response of heat current at resonant driving.

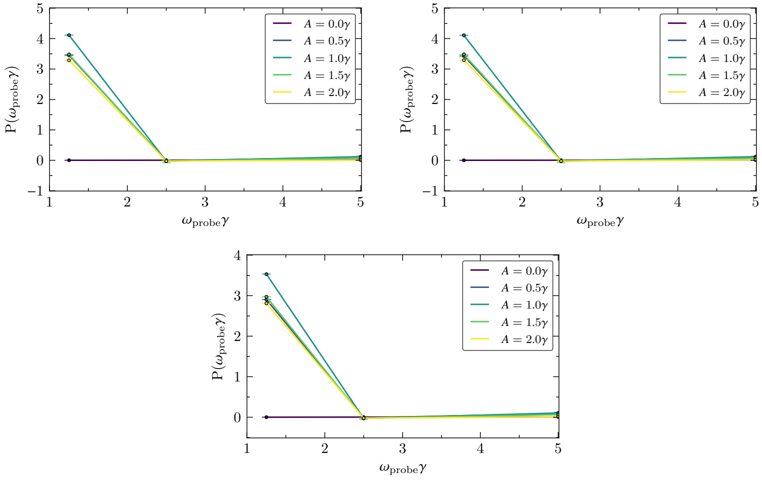

Figure 13: From left to right and top to bottom: $T = 0.06\gamma$, $T = 0.2\gamma$, $T = 1.0\gamma$

Results

Response of heat current at resonant driving.

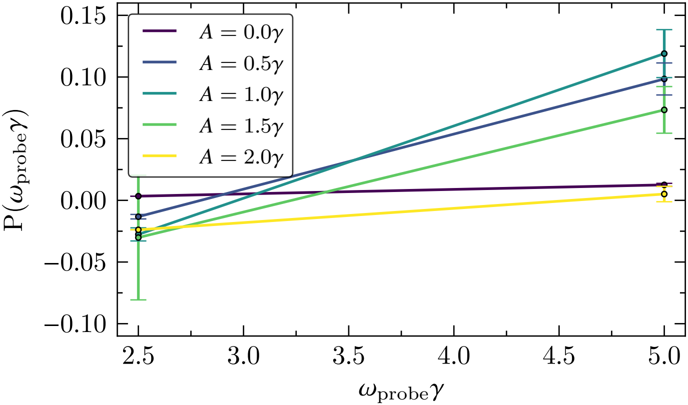

Figure 14: Zoom into $T = 0.06\gamma$

Results

Time evolution of spectral fuctions for various amplitudes at resonant driving.

$$G^{r}(t,t') = \Theta(t-t')(G^{>}(t,t') - G^{<}(t,t'))$$

$$A(\omega) = -\frac{1}{\pi}\mathrm{Im}G^{r}(\omega)$$

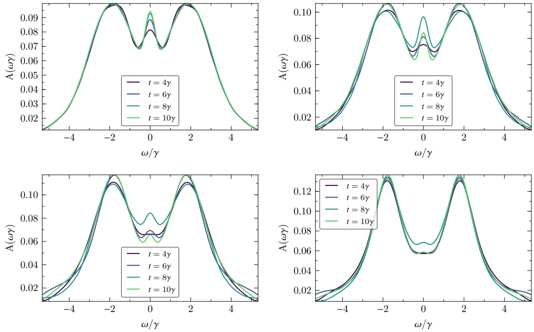

Figure 15: Time evolved spin-averaged spectral functions for $T = 0.06\gamma$. Top left $A_{ump} = 0.0$, top right $A = 0.5$, bottom left $A = 1.0$ and bottom right $A = 2.0$.

Results

Steady-state spectral fuctions for various amplitudes at resonant driving.

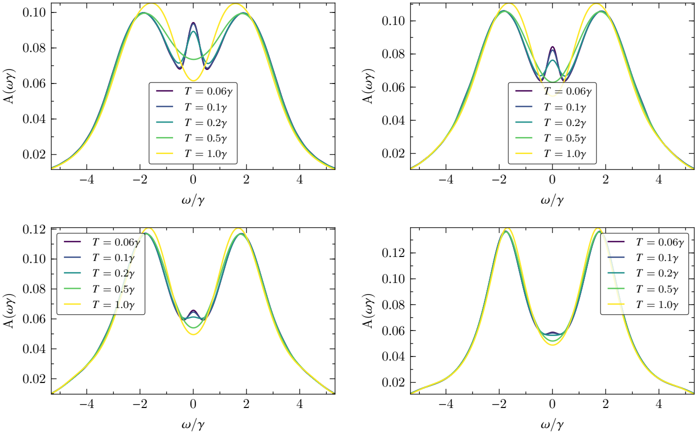

Figure 16: Spectral function averaged over initial spin up and spin down state. Top left $A = 0.0$, top right $A = 0.5$, bottom left $A = 1.0$ and bottom right $A = 2.0$.

Results

Response of heat current at half-resonant driving.

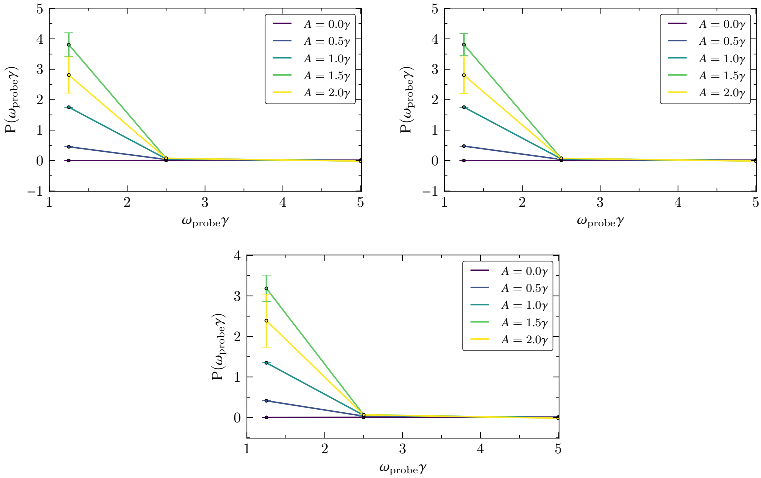

Figure 17: From left to right and top to bottom: $T = 0.06\gamma$, $T = 0.2\gamma$, $T = 1.0\gamma$

Results

Response of heat current at half-resonant driving.

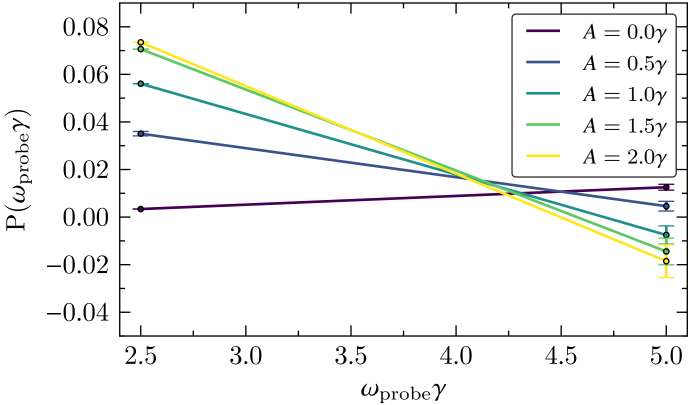

Figure 18: Zoom into $T = 0.06\gamma$

Results

Time evolution of spectral fuctions for various amplitudes at half-resonant driving.

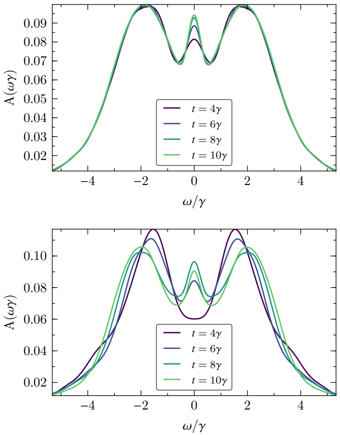

Figure 19: Time evolved spin-averaged spectral functions for $T = 0.06\gamma$. Top left $A_{ump} = 0.0$, top right $A = 0.5$, bottom left $A = 1.0$ and bottom right $A = 2.0$.

Results

Spectral fuctions for various amplitudes at half-resonant driving.

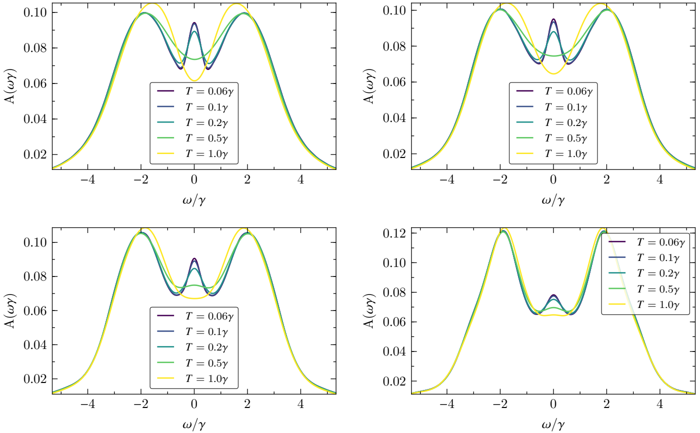

Figure 20: Spectral functions averaged over initial spin up and spin down state. Top left $A = 0.0$, top right $A = 0.5$, bottom left $A = 1.0$ and bottom right $A = 2.0$.