A LISA DMFT to study the Mott transition in the Hubbard model

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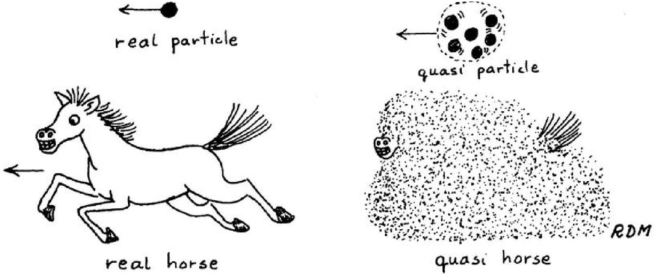
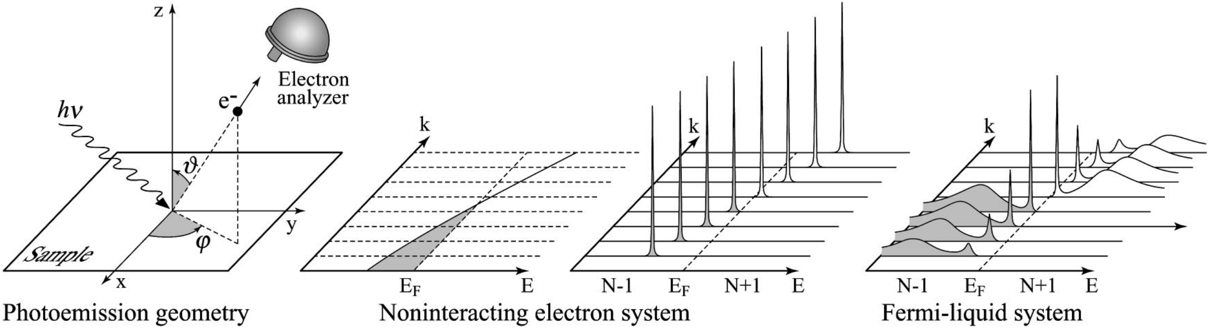
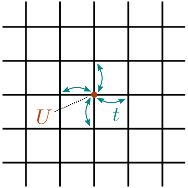
Introduction



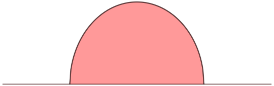


Hubbard Model

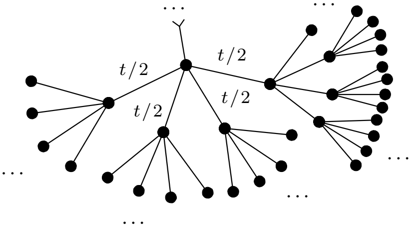


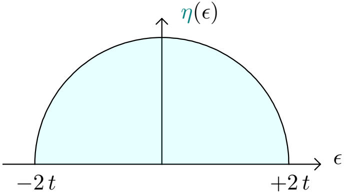
$$H = -\underbrace{\sum_{\langle i,j\rangle,\sigma} t_{ij}\left(c^{\dagger}_{i\sigma}c_{j\sigma} + c^{\dagger}_{j\sigma}c_{i\sigma}\right)}_{\text{hopping / hybridization}} + \underbrace{U\sum_{i} n_{i\uparrow}n_{i\downarrow}}_{\text{Coulomb repulsion}}$$

$\longrightarrow$ **Single orbital**



non-interacting VS **atomic** limit





$\longrightarrow$ **Infinite** dimension

$\longrightarrow$ **Bethe** lattice

$\longrightarrow$ **Half-filling**

$\longrightarrow$ **Finite** temperature

Green's function formalism

$\longrightarrow$ *zero-temperature time-ordered one-body Green's function*

$$G(i,t,j,t') = -\mathrm{i}\,\langle \mathrm{GS}|\, T c_i(t) c_j^\dagger(t')\, |\mathrm{GS}\rangle \text{ with } T \text{ time-ordering operator}$$

$\longrightarrow$ *finite-temperature Green's function in Matsubara time*

$$G_\beta(i,j,\tau) = \tfrac{1}{Z}\,\mathrm{tr}\Big(\mathrm{e}^{-\beta H_{\mathrm{GC}}}\, T c_i(\tau) c_j^\dagger(0)\Big) \text{ with } c(\tau) = \mathrm{e}^{H_{\mathrm{GC}}\tau} c\, \mathrm{e}^{-H_{\mathrm{GC}}\tau}$$

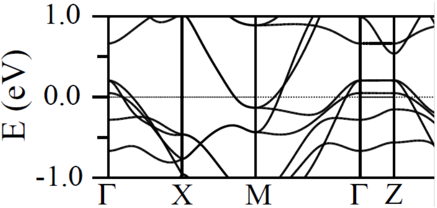
$\longrightarrow$ *relation between Matsubara Green's function and the spectral function*

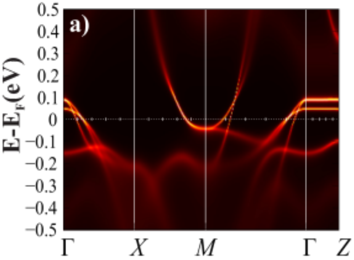
$$G_\beta(\tilde{k}, \mathrm{i}\omega_n) = \int_{-\infty}^{+\infty} \mathrm{d}\omega'\, \frac{A(\tilde{k},\omega')}{\mathrm{i}\omega_n - \omega'} \text{ with } \omega_n = \frac{2n+1}{\beta}\pi \text{ Matsubara frequencies}$$

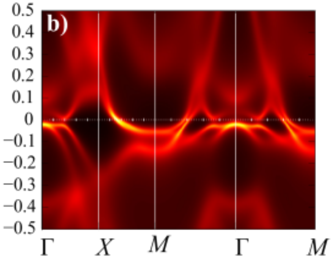
Self-energy

$$\text{Dyson equation}: \Sigma(\tilde{k}, i\omega_n) = G_0(\tilde{k}, i\omega_n)^{-1} - G(\tilde{k}, i\omega_n)^{-1}$$

$$\text{Interacting Green's function}: G(\tilde{k}, i\omega_n) = \frac{1}{i\omega_n - \epsilon(\tilde{k}) + \mu - \Sigma(\tilde{k}, i\omega_n)}$$







$LaFeAsO$
Weak interactions

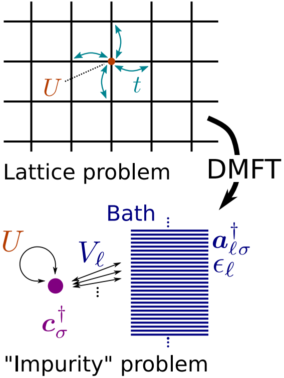
$LaFeAsO_{1x}H_x$
Strong interactions

Hypothesis of **infinite** dimension :
$\rightarrow$ *no more correlations betweens sites*
$\rightarrow$ *quantum fluctuations become purely local*
$\Longrightarrow$ *purely local self-energy*

$$\Sigma_{ij} \overset{\text{DMFT}}{\approx} \Sigma_{\text{loc}}\delta_{ij} \quad \Leftrightarrow \quad \Sigma(\tilde{k}) \approx \Sigma_{\text{loc}}$$

Mean field := two ingredients :

- **auxiliary system** $\longrightarrow$ impurity model
- **mean-field equation** $\longrightarrow$ implement symmetries



$\longrightarrow$ **Impurity model Hamiltonian :**

$$H^{\mathrm{GC}}_{\mathrm{imp}} = H_{\mathrm{site}} + H_{\mathrm{coupl}} + H_{\mathrm{bath}}$$

where

$$\begin{cases} H_{\mathrm{site}} = -\mu(n_\uparrow + n_\downarrow) + U n_\uparrow n_\downarrow \quad (n = c^\dagger c) \\ H_{\mathrm{bath}} = \sum_{\ell\sigma} E_\ell a^\dagger_{\ell\sigma} a_{\ell\sigma} \\ H_{\mathrm{coupl}} = \sum_{\ell\sigma} V_\ell (a^\dagger_{\ell\sigma} c_\sigma + c^\dagger_\sigma a_{\ell\sigma}) \end{cases}$$

$\longrightarrow$ **Self-consistency condition :**

local Hubbard $\rightarrow$ $G^{\mathrm{latt}}_{\mathrm{loc}} \overset{!}{=} G^{\mathrm{imp}}$ $\leftarrow$ impurity

$\longrightarrow$ **Bath equation :**

$$\mathcal{G}_0 = \text{Mean-Field}[G^{\mathrm{latt}}_{\mathrm{loc}}]$$

determine the dynamical mean field

$$\mathcal{G}_0 = \mathrm{DMF}[G_{\mathrm{loc}}]$$

$$\left(\mathcal{G}_0^{-1} = \Sigma_{\mathrm{loc}} + G_{\mathrm{loc}}^{-1} \text{ with } G_{\mathrm{loc}}(\mathrm{i}\,\omega_n) = {\sum_k}' \frac{1}{\mathrm{i}\omega_n - \epsilon_k + \mu - \Sigma(\mathrm{i}\omega_n)} \right)$$

solve the impurity problem

$$G^{\mathrm{imp}} = \mathrm{ImpuritySolver}[\mathcal{G}_0, U]$$

self-consistency

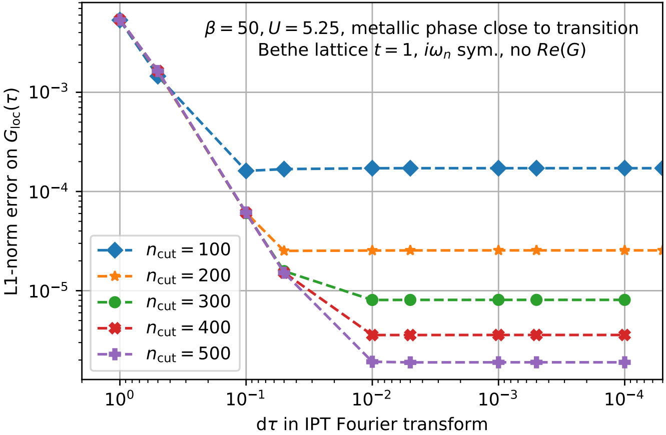
$$G_{\mathrm{loc}} \overset{!}{=} G^{\mathrm{imp}}$$

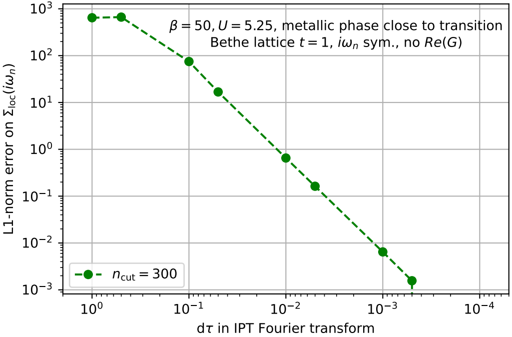
Iterated Perturbation Theory

$$\Sigma^{\text{imp}}(\mathrm{i}\omega_n) \simeq \frac{U}{2} + U^2 \int_0^\beta \mathrm{d}\tau\, e^{\mathrm{i}\omega_n\tau} \mathcal{G}_0'(\tau)^3 \quad \text{where} \quad \frac{1}{\mathcal{G}_0'(\mathrm{i}\omega_n)} = \frac{1}{\mathcal{G}_0(\mathrm{i}\omega_n)} - \frac{U}{2}$$

- Valid at *half-filling* only!
- Perturbative solution for non-interacting limit
- **In fact**, also exact at atomic limit, good in between.

Numerical implementation





Numerical implementation

Numerical implementation

An ill-posed inversion problem

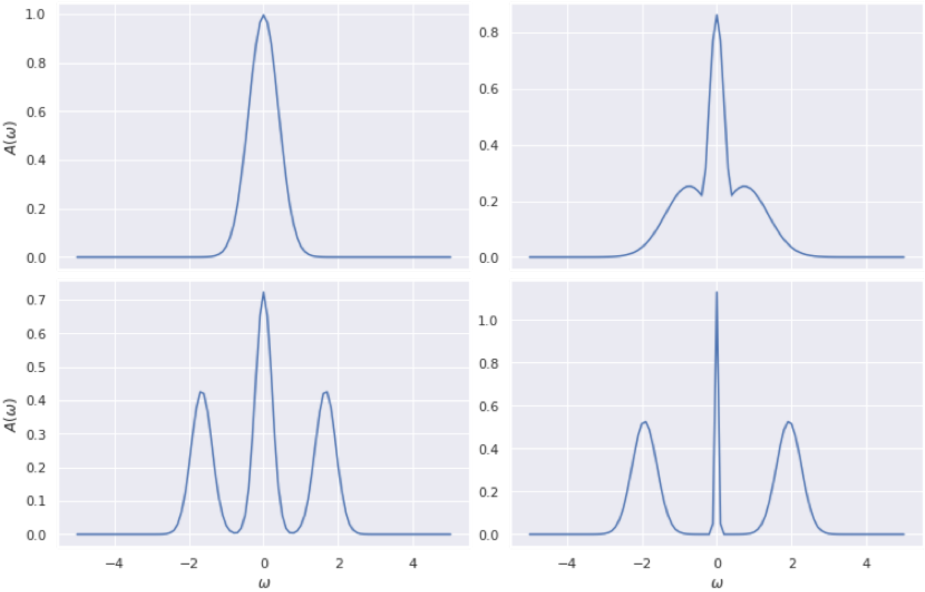
$$G_\beta(\tilde{k}, \mathrm{i}\omega_n) = \int_{-\infty}^{+\infty} \mathrm{d}\omega' \, \frac{A(\tilde{k}, \omega')}{\mathrm{i}\omega_n - \omega'}$$

- Inversion of a kernel: ill-posed problem;
- Learn a reconstruction $\rightarrow$ Machine Learning.

Training data

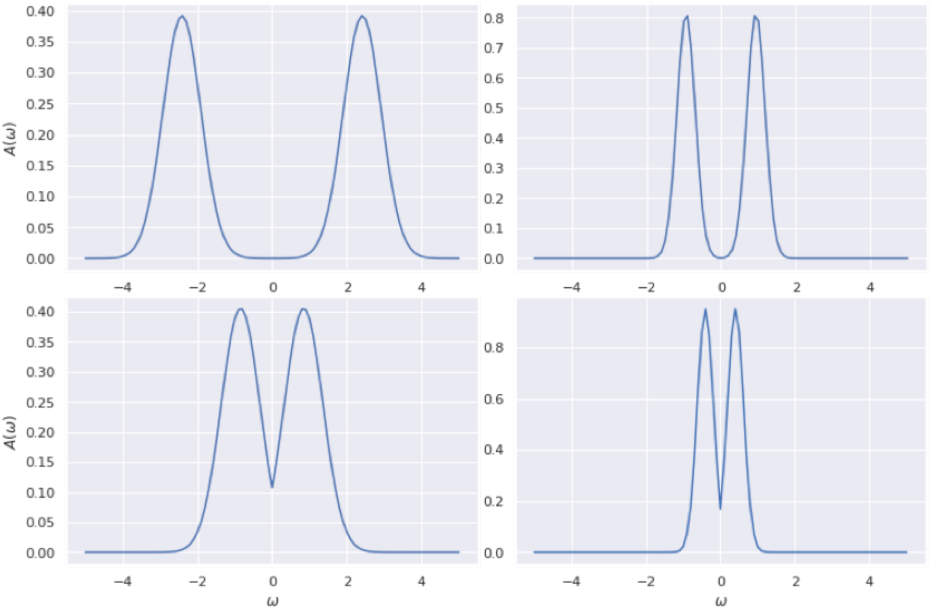
- Generate $A(\omega)$ with Gaussian peaks;
- Compute $A(\omega) \mapsto G(\mathrm{i}\omega_n)$;
- For the 1^{st} 300 frequencies;
- On 100 000 spectral densities.

Metals



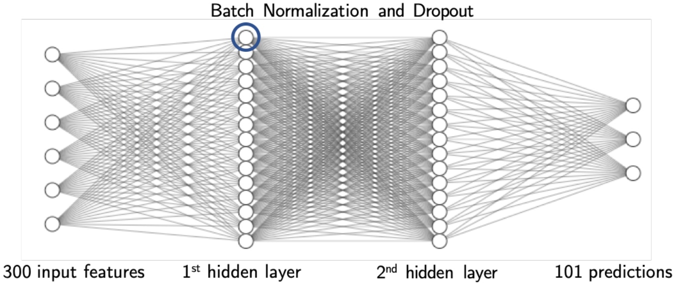
1.0
0.8
0.6
0.4
0.2
0.0
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
1.0
0.8
0.6
0.4
0.2
0.0
$A(\omega)$
$A(\omega)$
−4
−2
0
2
4
ω
−4
−2
0
2
4
ω

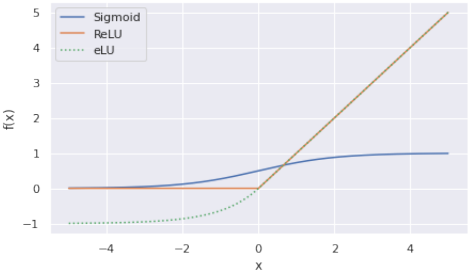
Insulators & bad metals



Neural Network

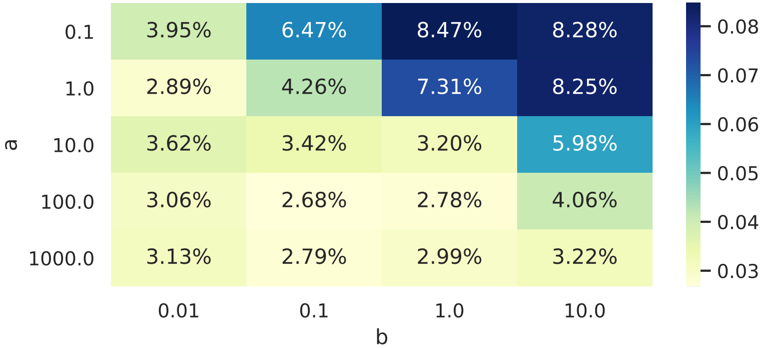
- Learning the weights and bias;
- Adam gradient descent;
- ReLU activation;
- 50% Dropout;
- 20 steps Early Stopping;
- Batch size of 128 samples.



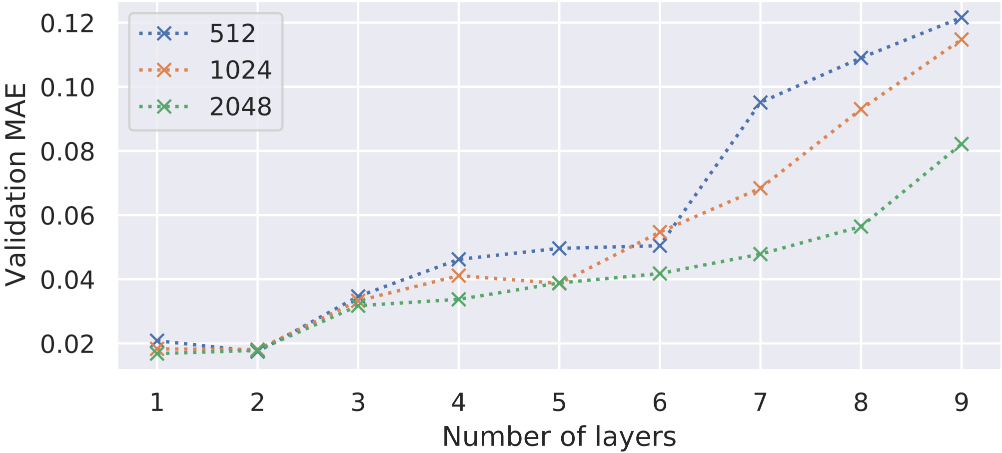


Custom loss

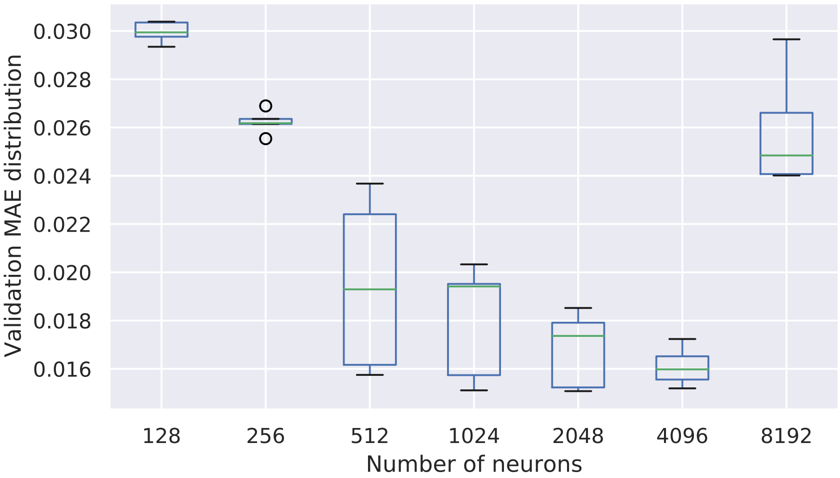
$$\ell(A, A_{\text{true}}) = a\|A - A_{\text{true}}\|_p + b\|\nabla_\omega A - \nabla_\omega A_{\text{true}}\|_p$$



Neural Network - Number of layers

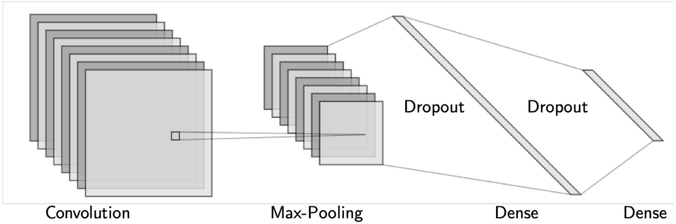


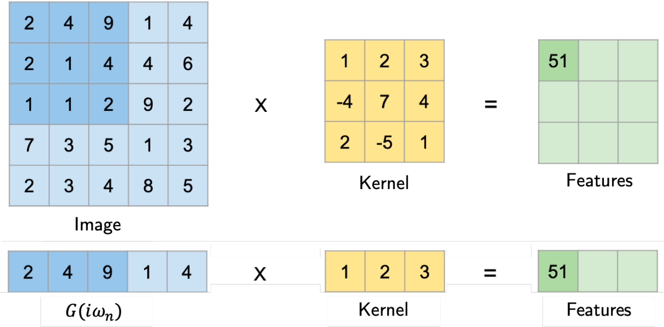
Neural Network - Number of neurons



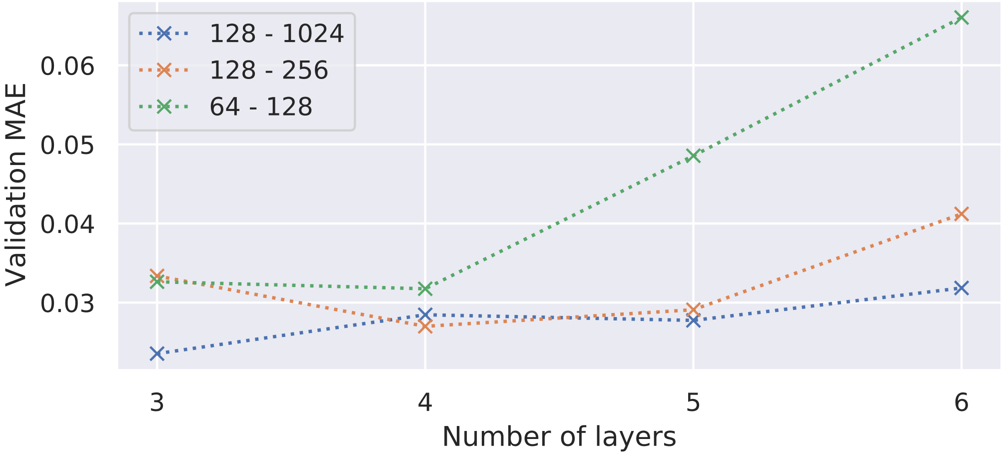
Convolutional Neural Network

- Exploit locality;
- Apply kernels on the input;
- Slower and bigger;
- Same optimization parameters;
- Similar investigation.

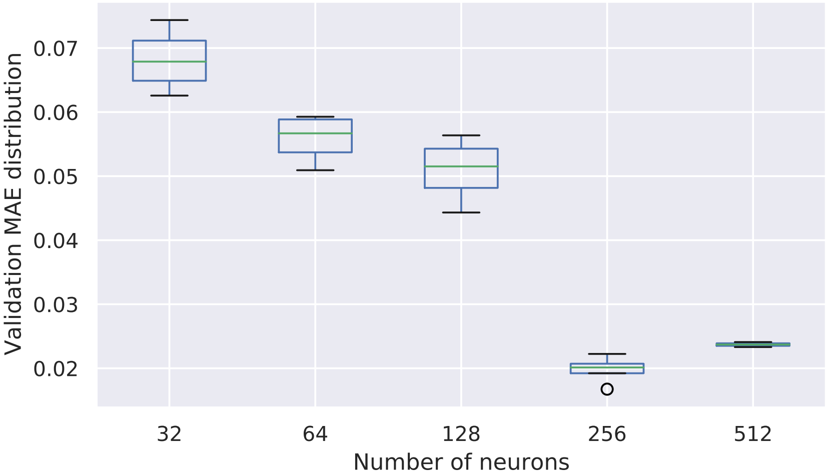




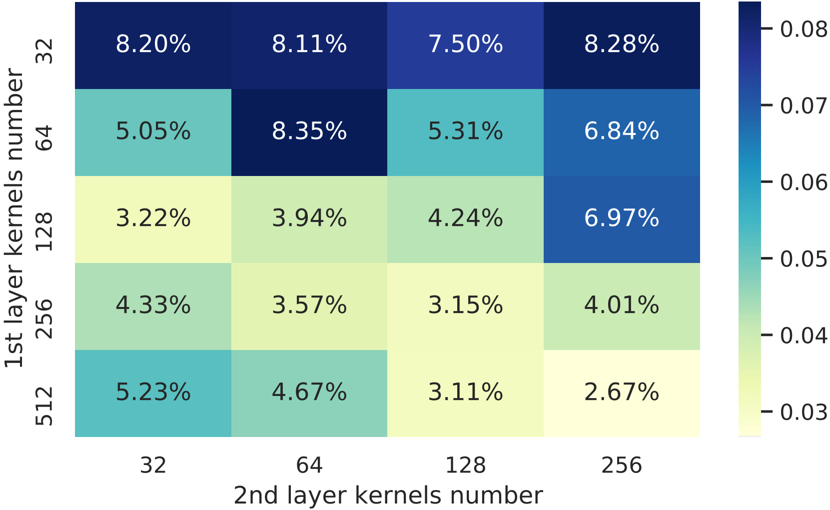
Convolutional Neural Network - Number of layers



Convolutional Neural Network - Number of kernels for 1 layer

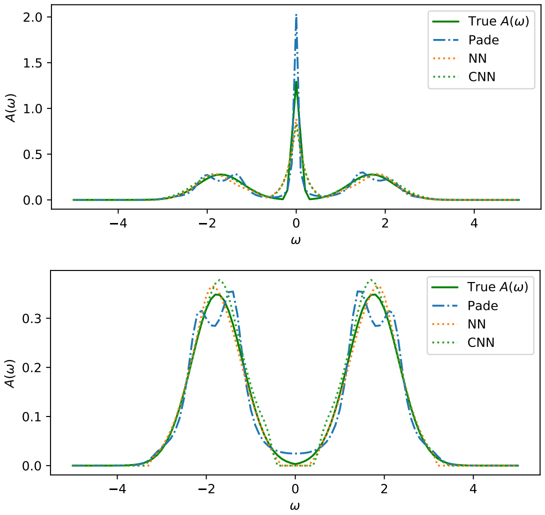


Convolutional Neural Network - Number of kernels for 2 layers



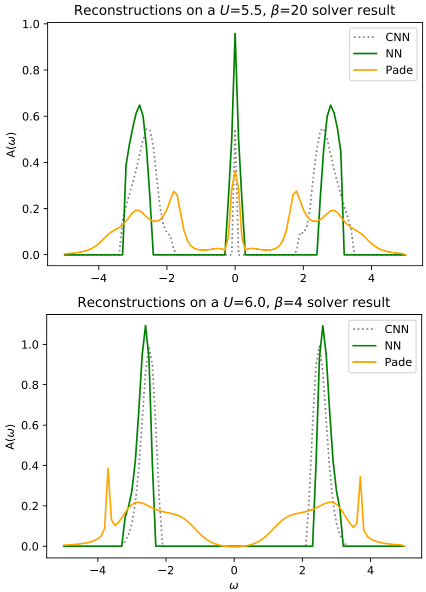
Best models

- Validation on 30 000 new densities;
- Padé: 2.28% MAE;
- Best NN: 1.44% MAE (-37%);
- Best CNN: 1.97% MAE (-11%);
- While 200% & 40% faster;
- 20Mo & 3.7Go.

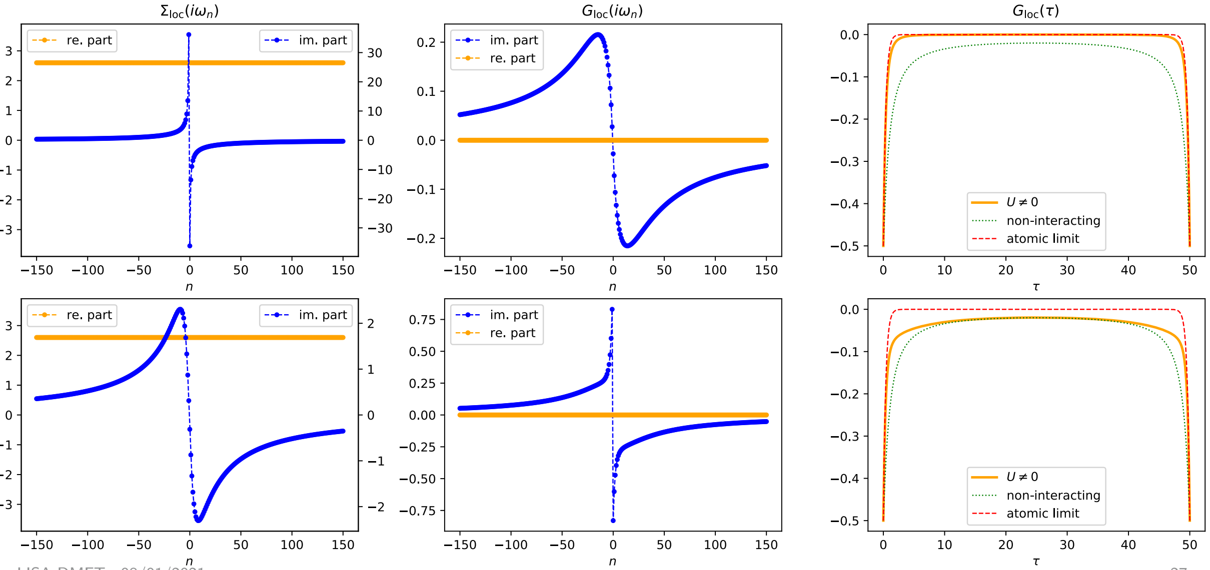


Models reconstruction

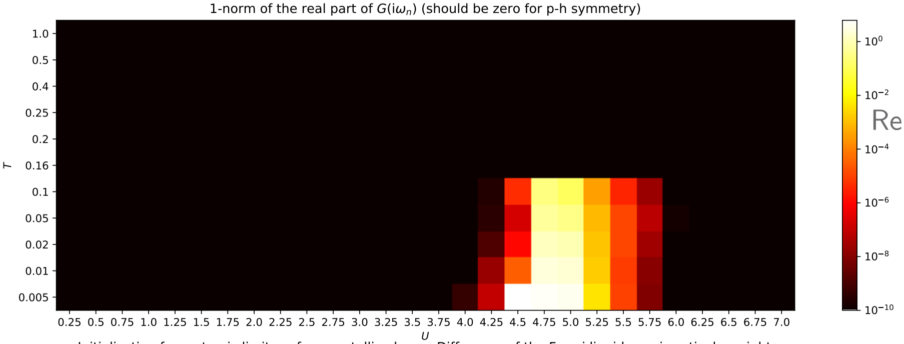
- Qualitative behavior reproduced;
- Incoherent peaks: position but wrong width;
- Wrong QP peak height $\rightarrow$ training data;
- Specific temperature training;
- Good learning on training data;
- Promising for improved data generation.



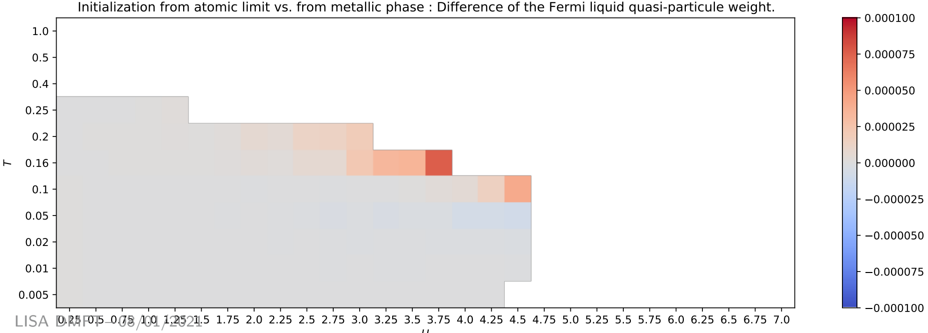
DMFT solution of the Hubbard model for $U = 5.2$, $\beta = 50$



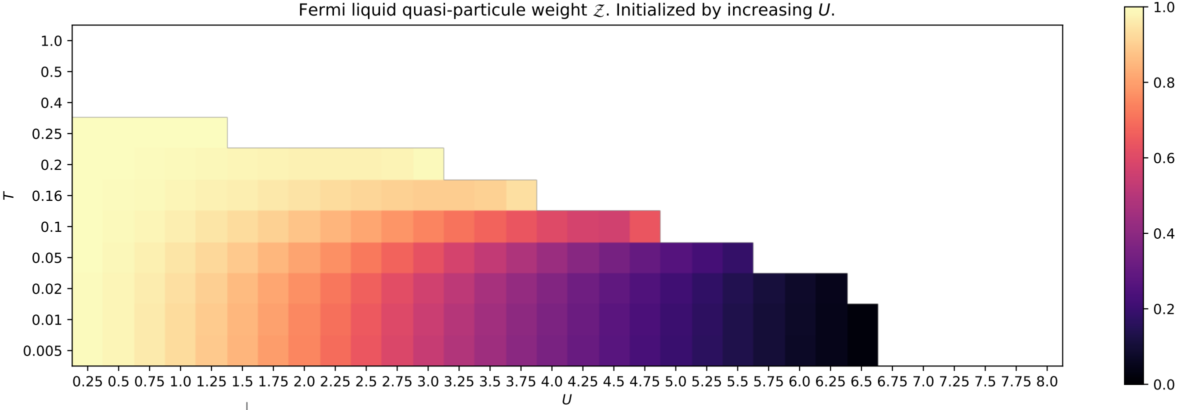
Sanity checks



$\mathrm{Re}\{G_{loc}(i\omega_n)\}$ unwanted!



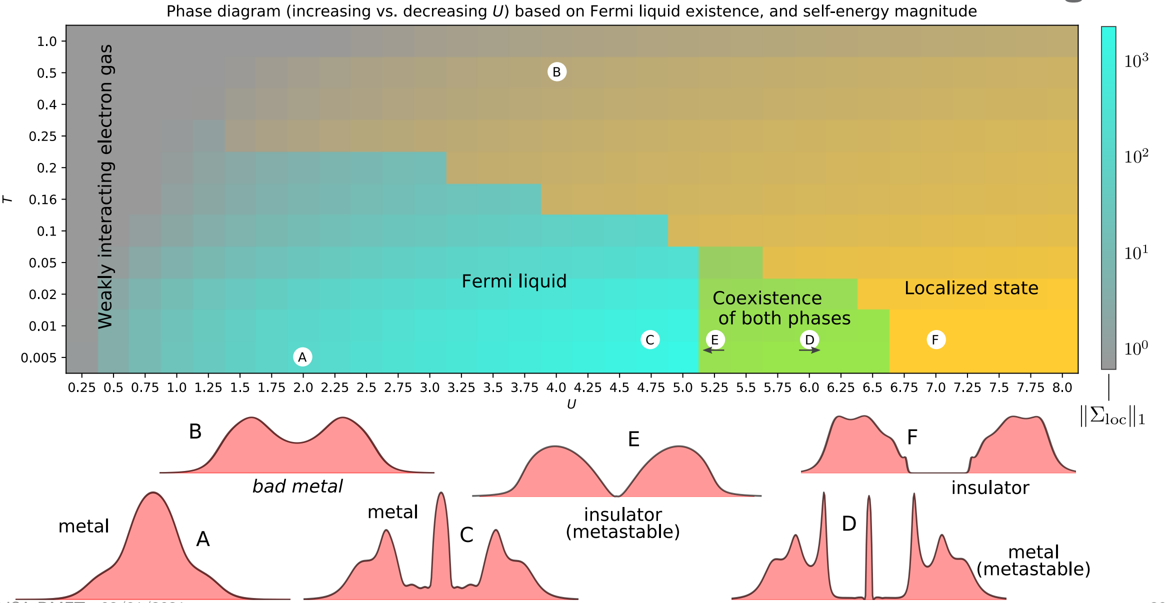
Fermi liquid



$$\mathcal{Z}_{\mathbf{k}}^{-1} = 1 - \left.\frac{\partial\Sigma(\tilde{k},z)}{\partial z}\right|_{z=0}$$

Fermi liquid phase when $\left.\frac{\partial\Sigma(\tilde{k},z)}{\partial z}\right|_{z=0} \geq 0$

Phase diagram



Momentum distribution for a cubic lattice