BACHELORARBEIT

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Verbreiterung von Spektralfunktionen des diskretisierten Single Impurity Anderson Model

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Broadening of spectral functions in the discretized single impurity Anderson model

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1 Introduction

Solving quantum many-body problems is usually difficult. Instead, one often tries to find essentially quantum mechanical models which mimic the original system. One of this models is the single impurity Anderson model proposed for magnetic impurities.

One way to solve the Anderson model approximately is to map the system onto a chain while preserving the impurity dynamics, thus getting an approximate chain representation of the Hamiltonian and then to diagonalize this object. While this idea can be made more sophisticated, it has one major disadvantage which we will consider in this thesis. The Anderson model has a continuous spectrum, arising from the coupling to a non-interacting bath of fermions[1].

However, in the process of iterative chain diagonalization, we necessarily approximate our system by a set of coupled few-level systems, which have a discrete spectrum!

What can be done is to artificially broaden this spectrum. While this can work well it has also serious shortcomings like the arbitrary nature of this broadening. There are some physical heuristics which serve as guidelines for how to broaden, but they do not lead to a unique description.

Therefore we will follow in this thesis an approach proposed by Frithjof Anders[1], on which i will rely through my hole thesis - to obtain an approximation to the spectrum of the system. It relies on neglecting correlations between the bath and the impurity. This is a priori a severe approximation and cannot rigorously be justified. However, correlations of an arbitrary high order can be incorporated into the scheme by considering longer chains, so one can hope for success. The corresponding algorithm will be explained and tested.

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[1]Since it is non-interacting, we will effectively solve quantum mechanical problems.

2   The Anderson Model For Magnetic Impurities

In this Section the model which will be studied is introduced

In the following we will only consider fermionic systems. The structure of the Hamiltonian is as following:

$$H = H^{imp} + H^{hyb} + H^{bath}_{-1}. \tag{1}$$

Next we introduce spin-$\frac{1}{2}$ annihilation operators, for the bath: $\{b_{\mathbf{k}-1\nu}\}$ and for the impurity $f_{-1\nu}$, subject to canonical anticommutation relations:

$$\{f_{n\nu}, f^{\dagger}_{m\mu}\} = \delta_{nm}\delta_{\nu\mu}; \quad \{b_{\mathbf{k}n\nu}, b^{\dagger}_{\mathbf{q}m\mu}\} = \delta_{nm}\delta_{\nu\mu}\delta_{\mathbf{kq}}. \tag{2}$$

The label "ν" shall label the spin-z-component, the label n denotes on which site we are, as will become clearer later when we will consider a system with several sites. For now, we set all labels $n = m = -1$, which is the label for the impurity site.

All other anticommutators are zero, and the anticommutator bracket $\{\cdot, \cdot\}$ for operators A,B is just given by

$$\{A, B\} = AB + BA.$$

We take as impurity Hamiltonian a spin-$\frac{1}{2}$ system with a on-site interaction, parametrized by a coupling U:

$$H^{imp} = H^{imp}_0 + V = \sum_{\nu=\uparrow\downarrow} \epsilon_{-1} f^{\dagger}_{-1\nu} f_{-1\nu} + U n_{\uparrow} n_{\downarrow}, \tag{3}$$

with the number operator $n_{\nu} = f^{\dagger}_{-1\nu} f_{-1\nu}$.

The other parts of the Hamiltonian are a hybridization term between the bath and the impurity

$$H^{hyb} = t_{-1} \sum_{\mathbf{k}\nu} \lambda_{\mathbf{k}-1\nu} b^{\dagger}_{\mathbf{k}-1\nu} f_{-1\nu} + h.c., \quad 1 = \sum_{\mathbf{k}} |\lambda_{\mathbf{k}-1\nu}|^2; \tag{4}$$

and the bath hamiltonian just describes a free band of conducting electrons:

$$H^{bath}_{-1} = \sum_{\mathbf{k}\nu} \epsilon_{\mathbf{k}} b^{\dagger}_{\mathbf{k}-1\nu} b_{\mathbf{k}-1\nu}. \tag{5}$$

In addition, we are free to choose t_{-1} real and positive, since any phase could be absorbed into the parameters λ.

Since the impurity couples only to a linear combination of bath modes, sometimes called the local bath operators, define

$$b_{-1\nu} = \sum_{\mathbf{k}} \lambda^{*}_{\mathbf{k}-1\nu} b_{\mathbf{k}-1\nu}. \tag{6}$$

This Hamiltonian has several symmetries we will exploit later; we will focus on two conserved quantities: the total number of particles and the z-component of the spin operator. They are given by

$$N = \sum_{\alpha} \left[f^{\dagger}_{-1\alpha} f_{-1\alpha} + \sum_{\mathbf{q}} b^{\dagger}_{\mathbf{q}-1\alpha} b_{\mathbf{q}-1\alpha} \right]$$

and

$$S_z = \sum_\alpha \alpha \left[f^\dagger_{-1\alpha} f_{-1\alpha} + \sum_{\mathbf{q}} b^\dagger_{\mathbf{q}-1\alpha} b_{\mathbf{q}-1\alpha} \right].$$

These are constants of motion, since $[H, S_z] = [H, N] = 0$, and since $[N, S_z] = 0$, we can find a simultaneous eigenbasis.

3   The Impurity Green's Function

Here we derive equations for the one-particle retarded Green's Function of the impurity. We drop this index, since for just one sign, there is no disambiguity. It will occasionally appear if a result is of importance for later sections.

A Green's function for general fermionic operators A, B is defined by:

$$\mathcal{G}^R_{A,B}(t - t') = -i\theta(t - t')\langle\{A, B\}\rangle_T, \tag{7}$$

here $\langle A\rangle_T = Tr\{\rho_\beta A\}$ denotes thermal averaging at inverse temperature[2] $\beta = \frac{1}{T}$ with the Gibbs State

$$\rho_\beta = \frac{e^{-\beta H}}{Z}, \quad Z = Tr\{e^{-\beta H}\}. \tag{8}$$

In particular, for the impurity:

$$\mathcal{G}^R_{f_\nu, f_\mu^\dagger}(t - t') = -i\theta(t - t')\langle\{f_\nu(t), f_\mu^\dagger(t')\}\rangle_T. \tag{9}$$

Since for a Hamiltonian as in Eq.(1) it is in general impossible to obtain the exact eigenstates, we will instead derive differential equations connecting different Green's functions.

3.1   Derivation of the Equations of Motion

We start by differentiating Eq.(9) w.r.t. time.

$$i\partial_t \mathcal{G}^R_{f_\nu, f_\mu^\dagger}(t - t') = \underbrace{(\partial_t\theta(t - t'))}_{\overset{(*)}{=}\delta(t-t')}\underbrace{\langle\{f_\nu(t), f_\mu^\dagger(t')\}\rangle_T}_{\delta_{\nu\mu}} +$$
$$- i\theta(t - t')\langle\{\underbrace{(i\partial_t f_\nu(t))}_{\overset{(\dagger)}{=}[f_\nu, H](t)}, f_{-1\mu}^\dagger(t')\}\rangle_T, \tag{10}$$

where at ($\dagger$) we used the Heisenberg equations of motion for not explicitly time-dependent operators

$$i\partial_t A(t) = [A(t), H(t)],$$

with the commutator bracket

$$[A, B] = AB - BA.$$

Due to Eq.(2) and the identity

$$[A, BC] = \{A, B\}C - B\{A, C\},$$

we can compute the equal-time-commutator appearing in Eq.(10):

$$[f_{-1\nu}, H] = \epsilon f_\nu + tb_\nu - Ud(\nu).$$

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[2] we work in units were $k_B = \hbar = 1$

Inserting this result in Eq.(10), the ODE for the impurity Green's Function reads:

$$i\partial_t \mathcal{G}^R_{f_\nu, f_\mu^\dagger}(t - t') = \delta_{\nu\mu}\delta(t - t') + \epsilon \mathcal{G}^R_{f_\nu, f_\mu^\dagger}(t - t') +$$
$$+ t\sum_{\mathbf{k}} \lambda^*_{\mathbf{k}\nu} \mathcal{G}^R_{b_{\mathbf{k}\nu}, f_\mu^\dagger}(t - t') + UD_{\nu\mu}(t - t'),$$

where we defined

$$d(\uparrow) = f_\uparrow n_\downarrow; \quad d(\downarrow) = f_\downarrow n_\uparrow;$$
$$D_{\nu\mu}(t - t') = \mathcal{G}^R_{d(\nu), f_\mu}(t - t').$$

By similar steps one obtains:

$$i\partial_t \mathcal{G}^R_{b_{\mathbf{k}\nu}, f_\mu^\dagger}(t - t') = \epsilon_{\mathbf{k}} \mathcal{G}^R_{b_{\mathbf{k}\nu}, f_\mu^\dagger}(t - t') + t\lambda_{\mathbf{k}\nu} \mathcal{G}^R_{f_\nu, f_\mu^\dagger}(t - t').$$

We introduce the Fourier transformation of a function f:

$$\mathcal{FT}[f](t) = \int \frac{d\omega}{2\pi} f(\omega) e^{-i(\omega - i\eta)t},$$

with the infinitesimal η ensuring convergence, it will usually not explicitly be displayed; furthermore we will usually denote the Fourier-transformed quantity by the same symbol as the original function.

By this integral transform a non-closed system of algebraic equations for the impurity Green's Function emerges:

$$(\omega - \epsilon)\mathcal{G}^R_{f_\nu, f_\mu^\dagger}(\omega) = \delta_{\nu\mu} + t\sum_{\mathbf{k}} \lambda^*_{\mathbf{k}\nu} \mathcal{G}^R_{b_{\mathbf{k}\nu}, f_\mu^\dagger}(\omega) + UD_{\nu\mu}(\omega)$$

$$(\omega - \epsilon_{\mathbf{k}})\mathcal{G}^R_{b_{\mathbf{k}\nu}, f_\mu^\dagger}(\omega) = t\lambda_{\mathbf{k}\nu} \mathcal{G}^R_{f_\nu, f_\mu^\dagger}(\omega). \tag{11}$$

More generaly, for operators A, B and a generator of the dynamics H we can write the equations of motion in Fourier base:

$$\omega \mathcal{G}^R_{A,B}(\omega) = \mathcal{FT}[\langle \{A(\cdot), B(\cdot)\}\rangle_T](\omega) + \mathcal{G}^R_{[A,H],B}(\omega). \tag{12}$$

The system of equations Eq.(11) can be simplified to

$$\mathcal{G}^R_{f_{-1\nu}, f_{-1\mu}^\dagger}(\omega) = \frac{\delta_{\nu\mu}}{\omega - \epsilon_{-1} - \Sigma_{-1\nu}(\omega)} + UD_{\nu\mu}(\omega), \tag{13}$$

where we have defined

$$|t_{-1}|^2 \sum_{\mathbf{k}} \frac{|\lambda_{\mathbf{k}-1\nu}|^2}{\omega - \epsilon_{\mathbf{k}}} =: \Sigma_{-1\nu}(\omega). \tag{14}$$

This object is called the bath self-energy due to the fact that it shifts the pole of the Impurity Green's function - and, through its imaginary part, also regularizes it[3]. The underlying reason for this is that the bath hamiltonian Eq.(5) is quadratic, so we can integrate its influence on the impurity out and obtain an effectively quantum-mechanical system, which will no longer possess a hamiltonian local in time.

It is worth stressing that $\Sigma_{-1\nu}$ appearing in Eq.(14) is not the full self-energy, since the interaction was not included.

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[3]The impurity Green's function fulfills an equation of the form $\partial_t \mathcal{G}^R(t) \propto \delta(t)$ and is thus a distribution.

3.2 Pertubative Solution

For now, we will go one step further in calculating Eq.(13) by searching for an equation for the Green's function $D_{\nu\mu}$. For simplicity, we set $\nu = \mu = \uparrow$, and drop the label -1 labeling that associates the operators with the impurity. Furthermore, we introduce the notation $(A, B)_\omega = G^R_{A,B}(\omega)$. Then $D_{\uparrow\uparrow}(\omega) = (f_\uparrow n_\downarrow, f^\dagger_\uparrow)_\omega$ fulfills the equation:

$$(\omega - \epsilon - U)(f_\uparrow n_\downarrow, f^\dagger_\uparrow)_\omega = \langle n_\downarrow \rangle_T + t(b_\uparrow n_\downarrow, f^\dagger_\uparrow)_\omega + t(f_\uparrow f^\dagger_\downarrow b_\downarrow, f^\dagger_\uparrow)_\omega - t(f_\uparrow b^\dagger_\downarrow f_\downarrow, f^\dagger_\uparrow)_\omega. \qquad (15)$$

We now assume that the bath is coupled only weakly to the impurity. This is, of course, a serious approximation and it is employed only since this is in fact the approximation we will mostly deal with in this thesis. This approximation treats the impurity exactly, while neglecting correlations with the bath.

This simplifies the above quantities:

$$(b_\uparrow n_\downarrow, f^\dagger_\uparrow)_\omega \approx \langle n_\downarrow \rangle_T (b_\uparrow, f^\dagger_\uparrow)_\omega - \langle f^\dagger_\downarrow b_\uparrow \rangle_T (f_\downarrow, f^\dagger_\uparrow)_\omega$$

$$(f_\uparrow f^\dagger_\downarrow b_\downarrow, f^\dagger_\uparrow)_\omega \approx -\langle f_\uparrow f^\dagger_\downarrow \rangle_T (b_\downarrow, f^\dagger_\uparrow)_\omega + \langle f^\dagger_\downarrow b_\downarrow \rangle_T (f_\uparrow, f^\dagger_\uparrow)_\omega$$

$$(f_\uparrow b^\dagger_\downarrow f_\downarrow, f^\dagger_\uparrow)_\omega \approx \langle b^\dagger_\downarrow f_\downarrow \rangle_T (f_\uparrow, f^\dagger_\uparrow)_\omega - \langle b^\dagger_\downarrow f_\uparrow \rangle_T (f_\downarrow, f^\dagger_\uparrow)_\omega$$

We could calculate from here, but in fact we will approximate further. Until now, the thermal expectation value $\langle \cdot \rangle_T$ was taken w.r.t. the full hamiltonian Eq.(1). Instead, we will now take it w.r.t. only the impurity hamiltonian Eq.(3), and we will take the limit of $T \to 0$. The latter is not necessary, but simplifies the analysis and furthermore will be the case studied throughout this thesis. With these approximations and convenient choices, our thermal averaging is just given by

$$\langle A \rangle_T = \frac{1}{\#} \sum_{\psi \in GS} Tr\{P_\psi A\},$$

where P_ψ is the projector onto the state ψ and $\psi \in GS$ should denote that we sum over the ground state, which may be degenerate with degeneracy $\#$.

It follows that the only non-vanishing object is

$$t(b_\uparrow n_\downarrow, f^\dagger_\uparrow)_\omega \approx \langle n_\downarrow \rangle_T t(b_\uparrow, f^\dagger_\uparrow)_\omega = \langle n_\downarrow \rangle_T \Sigma_\uparrow(\omega)(f_\uparrow, f^\dagger_\uparrow)_\omega$$

All other expectation values remain zero, since the thermal averaging is only taken w.r.t. the impurity hamiltonian, so not only the total number of particles, but also the number of particles in each of the subsystems has to be constant[4]. Additionally, every expectation value of a spin-changing operator will vanish, since we have simultaneous eigenstates of H and S_z.

Therefore, we have to solve:

$$\begin{pmatrix} \omega - \epsilon - \Sigma_\uparrow(\omega) & -U \\ -\langle n_\downarrow \rangle_T \Sigma_\uparrow(\omega) & \omega - \epsilon - U \end{pmatrix} \begin{pmatrix} (f_\uparrow, f^\dagger_\uparrow)_\omega \\ (f_\uparrow n_\downarrow, f^\dagger_\uparrow)_\omega \end{pmatrix} = \begin{pmatrix} 1 \\ \langle n_\downarrow \rangle_T \end{pmatrix}.$$

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[4]This is because the impurity number operator $N^{imp} = \sum_\alpha n_\alpha$ commutes with the impurity hamiltonian.

The solution has the following form:

$$(f_\uparrow, f_\uparrow^\dagger)_\omega = \frac{1 + \frac{U\langle n_\downarrow\rangle_T}{\omega - \epsilon_{-1} - U}}{\omega - \epsilon_{-1} - \Sigma_{-1\uparrow}(\omega)\left(1 + \frac{U\langle n_\downarrow\rangle_T}{\omega - \epsilon_{-1} - U}\right)}, \tag{16}$$

this functions has two very distinct appearance, depending on the ground state degeneracy.

- there is a degenerate ground state: this happens if $U > 0 > \epsilon_{-1}$ and $U > -\epsilon_{-1}$. We will investigate its properties later in Section 6.3.

- there is a unique ground state: this is in all other cases. Here, we can simplify Eq.(16), since $\langle n_\downarrow\rangle_T \in \{0, 1\}$, to

$$(f_\uparrow, f_\uparrow^\dagger)_\omega = \frac{1}{\omega - \epsilon_{-1} - \Sigma_{-1\uparrow}(\omega) - U\langle n_\downarrow\rangle_T}.$$

This means that at this level of the approximation, the only effect of the interaction is to shift the pole of the Green's function, if the state with one spin-down particle has the lowest eigenlevel.

4 Mapping Onto Semi-Infinite Chain

In principle we could try to solve Eq.(1), and there may be cases, where it is possible to obtain exact solutions, in fact we will later do one simple case. But for the general case, there is not much to hope. In the following section we will describe a method to replace our system by one better suited for numerical analysis, called Wilson chains, by a method proposed by Frithjof Anders.

Therefore, we start with an new Hamiltonian, having exactly the form of a resonant level mode. We will introduce new fermionic annihilation operators $\{b_{\mathbf{k}0\nu}\}_{\mathbf{k}\nu}$, which annihilate particles in a 2nd bath a priori unrelated to the first one, but subject to canonical anticommutation relations, furthermore define

$$f_{0\nu} = b_{-1\nu}.$$

We choose the Hamiltonian to be:

$$H_0^{bath} = \sum_{\mathbf{k}\nu} \epsilon_{\mathbf{k}} b_{\mathbf{k}0\nu}^\dagger b_{\mathbf{k}0\nu} + \sum_\nu \epsilon_{0\nu} f_{0\nu}^\dagger f_{0\nu} + \sum_\nu (t_{0\nu} b_{0\nu}^\dagger f_{0\nu} + h.c.);$$

$$b_{0\nu} = \sum_{\mathbf{k}} \lambda_{\mathbf{k}0\nu}^* b_{\mathbf{k}0\nu}, . \tag{17}$$

To fix the canonical normalization for the anticommutation relations for the $b_{0\nu}$, we have to impose $1 = \sum_{\mathbf{k}} |\lambda_{\mathbf{k}0\nu}|^2$. Note further that the local bath operators $b_{-1\nu} = f_{0\nu}$ appear in this expression, which will provide the link to our original system.

Set the new on-site-energy to be

$$\epsilon_{0\nu} = \sum_{\mathbf{q}} \epsilon_{\mathbf{q}} |\lambda_{\mathbf{q}-1\nu}|^2. \tag{18}$$

This follows if we require that the one-particle excitation has the same energy w.r.t. the new and the old bath Hamiltonian:

$$\epsilon_{0\nu} = \langle f_{0\nu}^\dagger \Omega, \epsilon_0 f_{0\nu}^\dagger f_{0\nu} f_{0\nu}^\dagger \Omega \rangle_0 = \langle f_{0\nu}^\dagger \Omega, H_0^{bath} f_{0\nu}^\dagger \Omega \rangle_0 \overset{!}{=} \langle b_{-1\nu}^\dagger \Omega, H_{-1}^{bath} b_{-1\nu}^\dagger \Omega \rangle_{-1} =$$

$$= \langle b_{-1\nu}^\dagger \Omega, \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} b_{\mathbf{k}-1\nu}^\dagger b_{\mathbf{k}-1\nu} b_{-1\nu}^\dagger \Omega \rangle_{-1} =$$

$$= \sum_{\mathbf{r},\mathbf{k},\mathbf{q}} \lambda_{\mathbf{r}-1\nu}^* \lambda_{\mathbf{q}-1\nu} \epsilon_{\mathbf{k}} \underbrace{\langle b_{\mathbf{k}-1\nu} b_{\mathbf{r}-1\nu}^\dagger \Omega}_{=\delta_{\mathbf{k}\mathbf{r}}\Omega}, \underbrace{b_{\mathbf{k}-1\nu} b_{\mathbf{q}-1\nu}^\dagger \Omega \rangle_{-1}}_{=\delta_{\mathbf{k}\mathbf{q}}\Omega} =$$

$$= \sum_{\mathbf{k}} |\lambda_{\mathbf{k}-1\nu}|^2 \epsilon_{\mathbf{k}}.$$

At the edges there are subscripts "-1" respectively "0", to indicate that these are the scalar products in the Hilbert space associated to the system sketched in Figure 1 a) and b) respectively. Furthermore Ω denotes the Fock vacuum, i.e. is annihilated by all annihilation operators.

We will restrict to the case that the bath couples equally to both spins, thus we will drop the spin-labels in the following. The formulas are not changed much if we would not do this,

since the spinorial part decouples from the dynamics for our non-interacting bath Hamiltonian, which has precisely the form of a resonant level mode.

We can now repeat the calculation leading us to Eq.(13), receiving

$$\mathcal{G}^R_{f_{-1\nu},f^\dagger_{-1\mu}}(\omega) = \frac{\delta_{\nu\mu}}{\omega - \epsilon_{-1} - \frac{|t_{-1}|^2}{\omega - \epsilon_0 - \Sigma_0(\omega)}} + U D_{\nu\mu}(\omega), \qquad (19)$$

where

$$\Sigma_0(\omega) = |t_0|^2 \sum_{\mathbf{k}} \frac{|\lambda_{\mathbf{k}0}|^2}{\omega - \epsilon_{\mathbf{k}}}. \qquad (20)$$

If we require that Eq.(13) and Eq.(19) agree, then it follows that

$$\Sigma_0(\omega) = \omega - \epsilon_0 - \frac{|t_{-1}|^2}{\Sigma_{-1}(\omega)}.$$

Our previous formulae allow a direct way for the computation of the on-site energy with aid of the self-energy, which will be useful in numerical implementation.

$$\frac{1}{\pi |t_{-1}|^2} \int d\omega \omega \Im\{\Sigma_{-1}(\omega - i\eta)\} \overset{(14)}{=} \frac{1}{\pi} \int d\omega \omega \Im \left\{ \sum_{\mathbf{k}} \frac{|\lambda_{\mathbf{k}-1}|^2}{\omega - \epsilon_{\mathbf{k}} - i\eta} \right\} =$$

$$= \int d\omega \omega \sum_{\mathbf{k}} |\lambda_{\mathbf{k}-1}|^2 \delta(\omega - \epsilon_{\mathbf{k}}) = \sum_{\mathbf{k}} |\lambda_{\mathbf{k}-1}|^2 \epsilon_{\mathbf{k}} \overset{(18)}{=} \epsilon_0,$$

where the relation $\frac{1}{x - i\eta} = \mathcal{P}\frac{1}{x} + i\pi\delta(x)$, with $\mathcal{P}$ the Cauchy principal value, was used for a positive infinitesimal η; and $\Im$ is the imaginary part. We can also compute $|t_0|^2$ out of Σ_0:

$$\frac{1}{\pi} \int d\omega \Im\{\Sigma_0(\omega - i\eta)\} \overset{(20)}{=} |t_0|^2 \sum_{\mathbf{k}} |\lambda_{\mathbf{k}0}|^2 \overset{(??)}{=} |t_0|^2$$

Starting from one impurity and a bath, we have deformed our system into one impurity, one additional site and a bath, which can be deformed again, iteratively, as sketched in Figure 1. We do so by recursions for the parameters t_n, ϵ_n and Σ_n. This also gives the hybridization constants, which we need for recursively defining new operators, by

$$\lambda_{\mathbf{q}n} = \frac{1}{\pi t_n^2} \lim_{\delta \to 0} \int_{\epsilon_{\mathbf{q}} - \delta}^{\epsilon_{\mathbf{q}} + \delta} d\omega \Im\{\Sigma_n(\omega - i\eta)\}.$$

So in each step, new operators

$$b_{n+1\nu} = \sum_{\mathbf{k}} \lambda^*_{\mathbf{k}n+1} b_{\mathbf{k}n+1\nu}, \quad 1 = \sum_{\mathbf{k}} |\lambda_{\mathbf{k}n+1}|^2, \quad b_{n\nu} = f_{n+1\nu} \qquad (21)$$

are introduced, and also operators for the new reservoir.

Let us fix the recursion relations: for this assume that we have constructed a chain from site
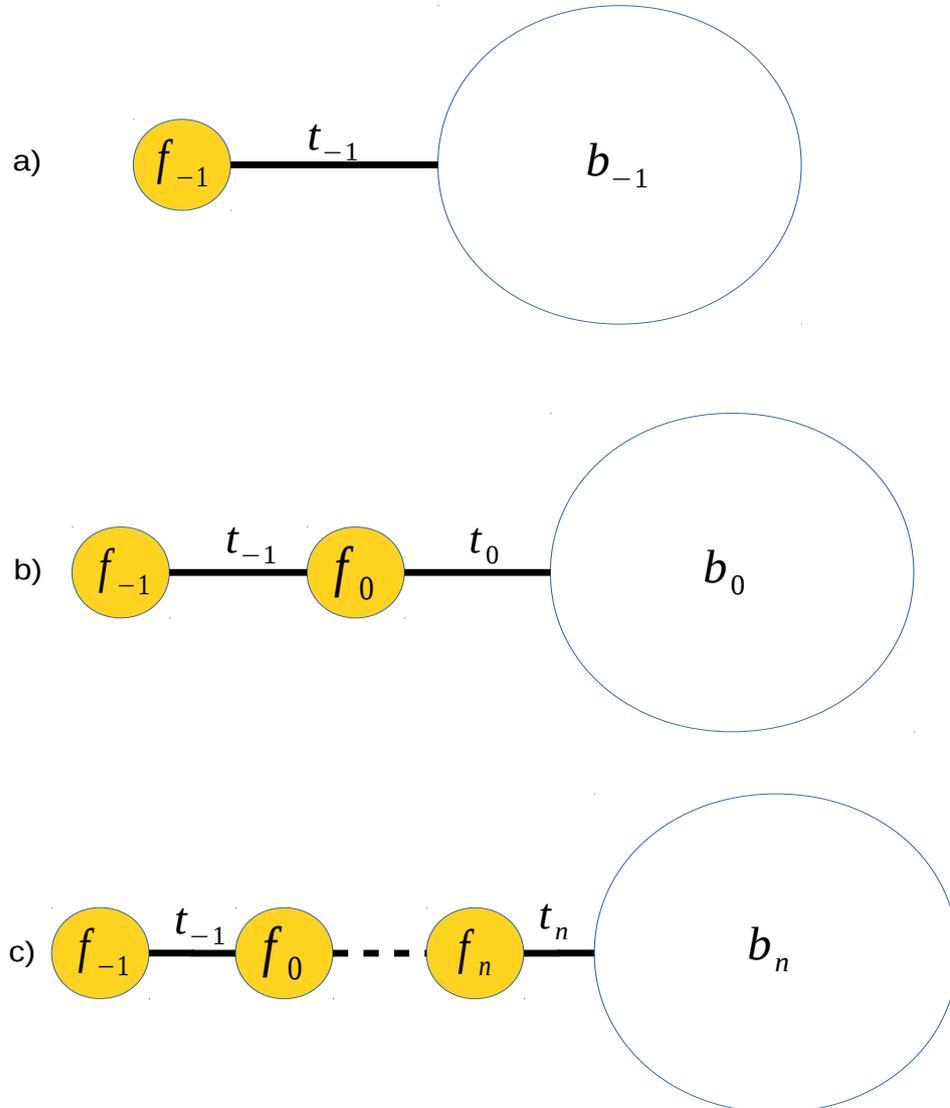
Figure 1: Here the procedure of iteratively constructing a chain is sketched. Yellow circles stand for sites, the larger empty circles are the baths, and the solid black lines are the hybridizations - over each the corresponding hybridization constant is written. In each circle the associated operator is written, but spin-indices are suppressed. a) describes the original system of one impurity, coupled to a bath. In b) we have added one additional site, while in c) the situation is shown after $n + 2$ steps, where at the dashed line intermediate sites are omitted in the picture.

-1 to site n already, so we know the quantities $\{\Sigma_k,\ t_k,\ \epsilon_k\}_{k=-1,\dots,n}$ and the Hamiltonian H_n. Then define the new on-site energy:

$$\epsilon_{n+1} = \frac{1}{\pi|t_n|^2}\int d\omega\,\omega\,\Im\{\Sigma_n(\omega - i\eta)\}. \tag{22}$$

The new self-energy:

$$\Sigma_{n+1}(\omega) = \omega - \epsilon_{n+1} - \frac{|t_n|^2}{\Sigma_n(\omega)}, \tag{23}$$

and the new hopping constant

$$|t_{n+1}|^2 = \frac{1}{\pi}\int d\omega\,\Im\{\Sigma_{n+1}(\omega - i\eta)\}. \tag{24}$$

The iterated chain Hamiltonian is then given by

$$H = \sum_{k=-1}^{n} H_k + H_n^B + \sum_{k=-1}^{n-1} H_{k,k+1}^{hyb} + H^I; \tag{25}$$

$$H_k = \sum_{\nu}\epsilon_k f_{k\nu}^\dagger f_{k\nu}, \quad H_k^B = \sum_{\mathbf{k}\nu}\epsilon_{\mathbf{k}} b_{\mathbf{k}n\nu}^\dagger b_{\mathbf{k}n\nu}, \quad H_{k,k+1}^{hyb} = t_k \sum_{\nu}(f_{k+1\nu}^\dagger f_{k\nu} + h.c.), \tag{26}$$

$$H^I = t_n \sum_{\nu}(b_{n\nu}^\dagger f_{n\nu} + h.c.), \tag{27}$$

and will generate the same impurity dynamics as Eq.(1). By reinserting all the parameters we have obtained, we can give a representation of the self-energy as an iterated fraction:

$$\Sigma_{-1}(\omega) = \cfrac{|t_{-1}|^2}{\omega - \epsilon_0 - \cfrac{|t_0|^2}{\omega - \epsilon_1 - \cfrac{|t_1|^2}{\omega - \epsilon_2 - \cfrac{|t_2|^2}{\ddots + \cfrac{|t_{n-1}|^2}{\omega - \epsilon_n - \Sigma_n(\omega)}}}}} \tag{28}$$

5 Lehmann-Representation Of The Spectral Function

We will now study a way to represent the spectral function in terms of its poles. The advantage of this method is that it will give a way to approximately compute the spectral function also for cases where the dynamics is not known - but this will not be done in this thesis.

In this section we will restrict to the case $U = 0$ and a special initial hybridization, in which case the answer is known and will be calculated in this section. From Eq.(13) we can read off that for $U = 0$ the spin degrees of freedom decouple and we can thus drop spinor indices.

5.1 Derivation Of The Lehmann-Representation For A Finite-Dimensional System

Given such an Hamiltonian Eq.(25), we can cut off the terms connecting the last reservoir coupling to chain site n Eq.(27). Now the bath decouples from the chain, so we can write down an approximate Hamiltonian:

$$H_n^{approx} = \sum_{k=-1}^{n} H_k + \sum_{k=-1}^{n-1} H_{k,k+1}^{hyb} \tag{29}$$

This is just a self-adjoint matrix and thus there is no substantial problem in diagonalizing it. Hence assume we have diagonalized H_n^{approx}, with Eigenvalues $\{E_k\}_{k=1,\dots n}$ and Eigenvectors $\{v_k\}_{k=1,\dots,n}$. We then introduce the so called Hubbard operators $X_{kl} = |k\rangle \otimes \langle l|$ with Projection operators $P_k = X_{kk}$ on the diagonal. In terms of these operators thermal averaging w.r.t. the approximate Hamiltonian Eq.(29) is given by $\langle A \rangle_T = \sum_k e^{-\beta E_k} Tr\{A P_k\} = \sum_k e^{-\beta E_k} (A)_{kk}$ with the matrix element $(A)_{kl} = Tr\{A X_{lk}\}$. Then we can give after short computation an exact expression for the approximated Green's function:

$$\begin{aligned}
\mathcal{G}^R_{f_{-1}, f_{-1}^\dagger}(t - t')\Big|_n &= -i\theta(t - t')\langle\{f_{-1}(t), f_{-1}^\dagger(t')\}\rangle_T = \\
&= -i\theta(t - t')\frac{1}{Z}\sum_k e^{-\beta E_k}(\{f_{-1}(t), f_{-1}^\dagger(t')\})_{kk} = \\
&= -i\theta(t - t')\frac{1}{Z}\sum_{k,l} e^{-\beta E_k}((f_{-1}(t) P_l f_{-1}^\dagger(t'))_{kk} + \\
&\quad + (f_{-1}^\dagger(t') P_l f_{-1}(t))_{kk}) = \\
&= -i\theta(t - t')\frac{1}{Z}\sum_{k,l} e^{-\beta E_k}((f_{-1}(t))_{kl}(f_{-1}^\dagger(t'))_{lk} + \\
&\quad + (f_{-1}^\dagger(t'))_{kl}(f_{-1}(t))_{lk}) = \\
&\overset{\dagger}{=} -i\theta(t - t')\frac{1}{Z}\sum_{k,l}(e^{-\beta E_k} + e^{-\beta E_l})e^{iE_{kl}(t-t')}|(f_{-1})_{kl}|^2,
\end{aligned}$$

where at (†) we used that $|k\rangle_T$ is a eigenvector of the Heisenberg dynamics, defined $E_{kl} = E_k - E_l$ and interchanged the summation indices k and l in the last term.

Taking the Fourier transform results in:

$$\mathcal{G}^R_{f_{-1},f^\dagger_{-1}}\bigg|_n = \frac{1}{Z}\sum_{k,l}(e^{-\beta E_k}+e^{-\beta E_l})|(f_{-1})_{kl}|^2 \frac{1}{\omega - E_{lk} - i\eta}.$$

Now we introduce a new concept, the so called spectral function or spectral weight, associated to every Green's function in the following way:

$$A = \frac{1}{\pi}\Im\mathcal{G}$$

. The normalization is chosen s.t. A fulfills a sum rule:

$$\int d\omega A(\omega) = 1.$$

So for the impurity Green's function we obtain:

$$A(\omega)\bigg|_n = \frac{1}{\pi}\Im\mathcal{G}^R_{f_{-1},f^\dagger_{-1}}(\omega)\bigg|_n =$$
$$= \frac{1}{Z}\sum_{k,l}(e^{-\beta E_k}+e^{-\beta E_l})|(f_{-1})_{kl}|^2\delta(E_{lk}-\omega). \tag{30}$$

Eq.(30) is a so called Lehmann Representation of the spectral function[5]. A special case of the formula derived above - which we will use for the rest of our numerical treatment - is the case of zero temperature or $\beta \to \infty$. Then

$$\frac{e^{-\beta H^{approx}_n}}{Z} \to \frac{1}{\#}\sum_{\alpha \in GS} P_\alpha,$$

where $\#$ is the degeneracy of the ground state and the sum is over the ground-subspace; so finally Eq.(30) simplifies to:

$$A(\omega)\bigg|_{n,T=0} = \frac{1}{\#}\sum_k \sum_{\alpha \in GS}(|(f_{-1})_{k\alpha}|^2\delta(E_{k\alpha}-\omega) + |(f_{-1})_{\alpha k}|^2\delta(E_{\alpha k}-\omega)). \tag{31}$$

5.2 Exact Solution For Non-Interacting Resonant Level Mode

The quantum impurity model from Eq.(1) is in general already complicated enough to resist attempts of solving it exactly analytically. So instead, since we focused on a toy model where exact results can be obtained, called the non-interacting resonant level mode, we can get explicit expressions for the Green's functions and then compare them with numerical calculations, thus

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[5]This is quite a general object and can also be defined for the unapproximated Green's function - but there the Gibbs state Eq.(8), which we used here, becomes more difficult due to the possibly continuous spectrum of the Hamiltonian in this case, which may or may not make the analysis harder. Since we will not need the full, infinitely-many-degrees-of-freedom case in this thesis, we just considered the easy case of finite dimensions with a discrete spectrum of the Hamiltonian.

testing the algorithms. We want to make Eq.(13) explicit by computing Eq.(14) for a special set of parameters. In the continuum limit, the self-energy can be written as:

$$\Sigma_{-1}(\omega - i\eta) = |t_{-1}|^2 \sum_{\mathbf{k}} \frac{|\lambda_{\mathbf{k}-1}|^2}{\omega - \epsilon_{\mathbf{k}} - i\eta} \to |t_{-1}|^2 \int d\epsilon \rho(\epsilon) \frac{1}{\omega - \epsilon - i\eta},$$

To go any further, we need to specify the hybridization. We choose the hybridization such that ρ is box-shaped:

$$\rho(\epsilon) = \begin{cases} \frac{1}{2} & \text{for } \epsilon < D \\ 0 & \text{else} \end{cases},$$

where D is the band width. In this case, we get for the selfenergy:

$$\Sigma_{-1}(\omega - i\eta) = -|t_{-1}|^2 \frac{1}{2} \log\left(\frac{\omega - D - i\eta}{\omega + D - i\eta}\right). \tag{32}$$

5.3 Numerical Tests for Resonant Level Mode

In this section, we will implement the recursion defined in Eq.(22) - Eq.(25) numerically for small chain lengths and the Resonant Level Mode solved in Eq.(32) . We will then arrive at the problem of how to smooth a dirac comb, which is the motivation for the topic of my thesis. In particular, in our studies, we start with a Bath Spectral Function as following:

$$A^B(\omega) = \begin{cases} 1 & \text{for } \omega < 1 \\ 0 & \text{else} \end{cases}, \tag{33}$$

from which we can deduce the self-energy by the Kramers-Kronig relation:

$$\Sigma_{-1}(\omega) = |t_{-1}|^2 \frac{1}{\pi} \int \frac{A^B(\omega')}{\omega - \omega' - i\eta} d\omega'.$$

That done, we apply the steps Eq.(22) to Eq.(24) to obtain the chain parameters $\{\epsilon_k, t_k\}_{k=-1,...n}$. Next, by using Eq.(26) and Eq.(29), we can get an explicit expression for H_n^{approx} as a matrix in the following way:
we define an one degree of freedom annihilation operator

$$d = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix},$$

by which we defined $(1,0)^\top$ as the one-degree-of-freedom operator corresponding to occupied site and $(0,1)^\top$ as the vector corresponding to an empty site.
For the chain Fock space operators we have to take into account the fact that we are dealing with fermions, thus we want our states antisymmetric under exchange of particles. Therefore, we define

$$Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

To be very explicit, we can now obtain the Fock operators by tensoring over the columns of the following matrix:

$$O = \begin{pmatrix} 1 & 1 & \ldots & 1 & d \\ 1 & 1 & \ldots & d & Z \\ \vdots & \vdots & \ddots & & \vdots \\ 1 & d & \ldots & Z & Z \\ d & Z & \ldots & Z & Z \end{pmatrix}.$$

So, for example :

$$f_{-1} = \bigotimes_{k=-1}^{n} (O)_{k,-1}.$$

For later convenience, we will also explain the representation of spin-$\frac{1}{2}$ creation and annihilation operator algebras as matrices by the same method. For that we define

$$Z_\uparrow = 1 \otimes Z; \quad Z_\downarrow = Z \otimes 1.$$

Here the 2x2-identity matrices were denoted by 1. Also, we introduce

$$d_\uparrow = 1 \otimes d; \quad d_\downarrow = d \otimes Z.$$

Consider

$$O_\uparrow = \begin{pmatrix} Z_\uparrow & Z_\uparrow & \ldots & Z_\uparrow & d_\uparrow \\ Z_\uparrow & Z_\uparrow & \ldots & d_\uparrow & Z_\downarrow \\ \vdots & \vdots & \ddots & & \vdots \\ Z_\uparrow & d_\uparrow & \ldots & Z_\downarrow & Z_\downarrow \\ d_\uparrow & Z_\downarrow & \ldots & Z_\downarrow & Z_\downarrow \end{pmatrix},$$

and similarly with all spins reversed for the spin down operators. As before, we take the tensor product over the columns.

Now, since we gave meaning to all chain operators in Eq.(26), the Hamiltonian H_n^{approx} of Eq.(29) is a very concrete self-adjoint matrix and we can therefore diagonalize it, feed the resulting eigenvectors and eigenenergies into Eq.(31) and obtain thus an approximation to the spectral function.

It is exactly at this point, that we have to employ some broadening to the spectral measure, since otherwise we are describing a set of discrete states, not the thermodynamic limit. There are many possible ways to do so, I convoluted it with a Lorentz peak:

$$L_\delta(x) = \frac{\delta/2}{\pi} \frac{1}{x^2 + (\delta/2)^2}. \tag{34}$$

The results are plotted in Figure 2. To be specific, the y-axis is the frequency ω, and on the x-axis, there is one the one hand the exact solution, obtained by plugging Eq.(32) into Eq.(13),

on the other hand the regularized spectral function $(L_\delta * A\big|_n)(\omega)$,for $n = k - 2$ sites, where k is the number of recursions displayed in the figure. The other parameter in the legend is exactly the parameter δ of our mollifier L_δ.

It changes in Figure 2 from iteration to iteration, since it is related to the matrix element $|(f_{-1})_{\alpha k}|^2$, which has a peak structure as well, say at positions $\{r_i\}_{i=1,M}$, then the broadening parameter δ is given by

$$\delta = \kappa \frac{\sum_{i=1}^{M} r_i}{M}. \tag{35}$$

Here, κ is a number of order unity, which is chosen such that the singularities of Eq.(31) disappear, but as close to one as possible.

In Figure 3, the parameter δ was chosen constant, such that there are no peaks visible and as small as possible. It is for these chain lengths not significantly better or worser.

The procedure outlined above serves as a good motivation for the procedure to come, for the way it was done here, the computation of the approximate Green's Function required three mostly arbitrary choices, and while there are some heuristics for some of them, there are really no derivations from first principles here. In the section to come, we will talk about a method of systematically computing the broadened spectral functions, without invoking arbitrary parameters.

Some remarks about the Figures itself: there seems to be an approach of the approximated Spectral Functions to the exact result with increasing chain length, but it is not clear if there is a convergence. The big problem here is that $L_\delta * A\big|_n$ has only possibility to converge to the true result if the chain length $n \to \infty$, which is not possible with a naive implementation of the Hamiltonian (Eq.29), since the size of the resulting matrix scales as d^{n+2}, where d is the number of degrees of freedoms at one site, so 2^{n+2} in our case.
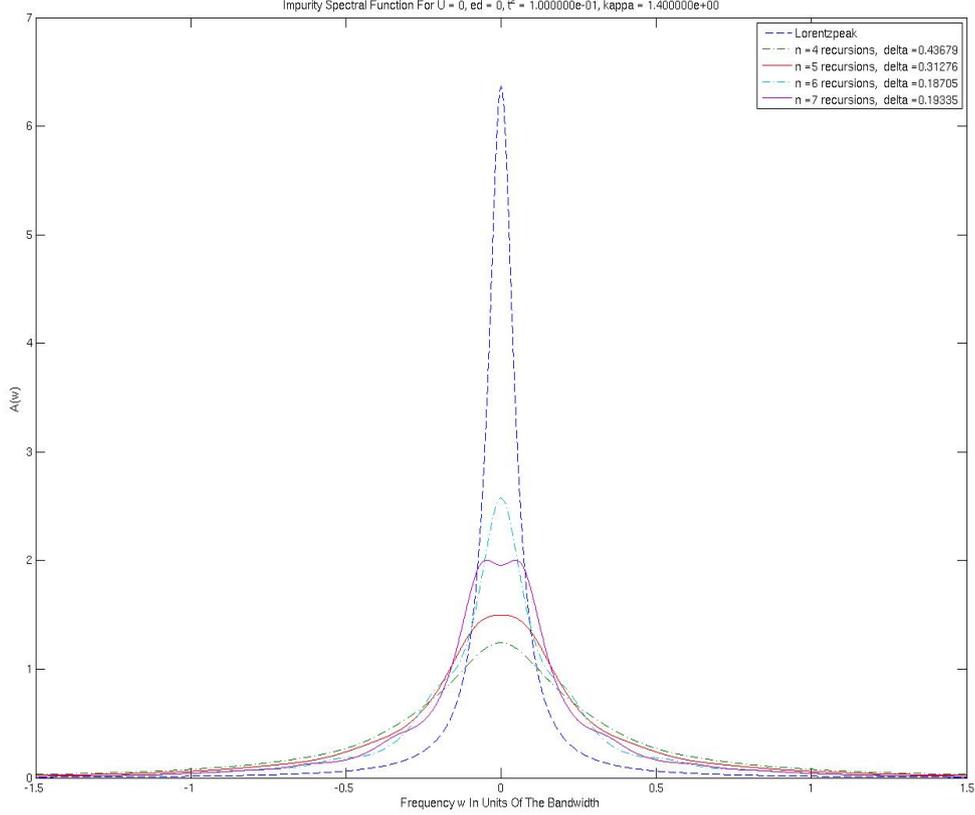
Figure 2: The plotted Lorentz peak is the exact solution corresponding to the insertion of Eq.(32) into Eq.(13), and then taking the imaginary part, $A(\omega) = \Im \mathcal{G}^R_{f_{-1}, f^\dagger_{-1}}$ with the system parameters $t^2_{-1} = 0.1$, $U = \epsilon_{-1} = 0$. The other curves are approximated impurity spectral functions $A(\omega)\big|_n$, given by Eq.(31), plotted for $n = 4, 5, 6, 7$, where the poles have been removed by convolution with L_δ given in Eq.(34), where delta is given for each of these curves in the legend, again all measured in units of the bandwidth. The procedure for obtaining δ is described in Eq.(35). The approximated spectral functions do not approximate the spectral function well. Nevertheless, there is a slight increase in the approximation for increasing n; but we have to take an even-odd effect into account: for n odd, $A(\omega)\big|_n$ has poles symmetric around zero - one can observe some traces of this for $A(\omega)\big|_7$. This worsens the convergence further.
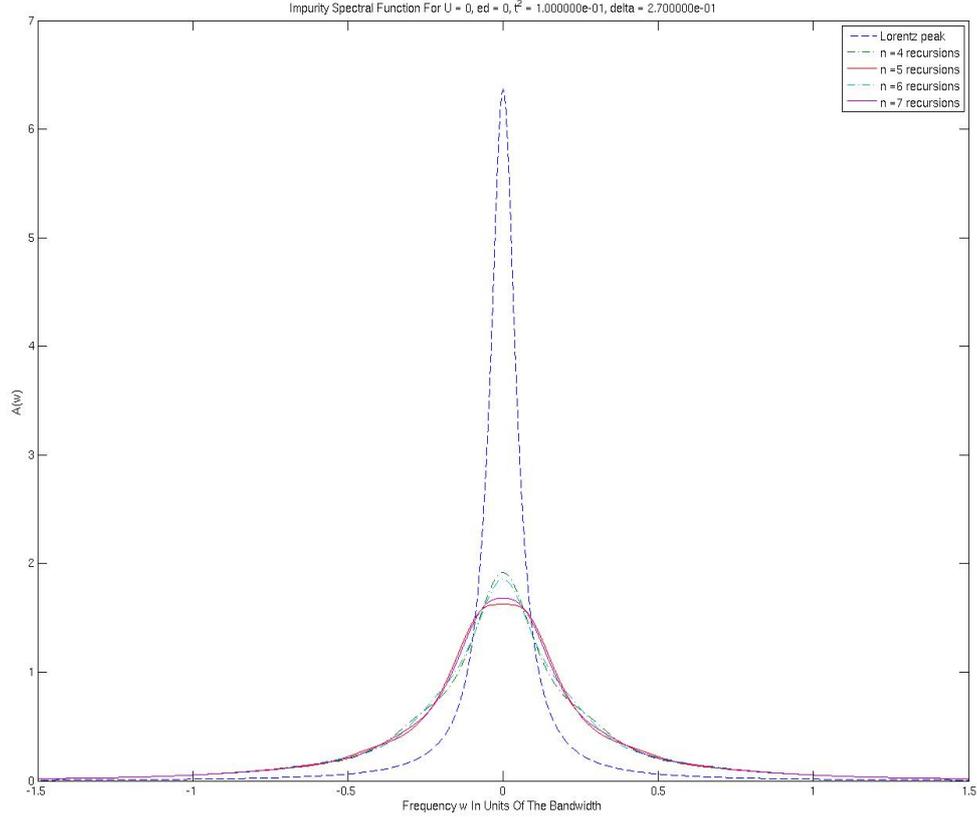
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Figure 3: The plotted Lorentz peak is the exact solution corresponding to the insertion of Eq.(32) into Eq.(13), and then taking the imaginary part, $A(\omega) = \Im \mathcal{G}^R_{f_{-1}, f^\dagger_{-1}}$ with the system parameters $t^2_{-1} = 0.1$, $U = \epsilon_{-1} = 0$. The other curves are approximated impurity spectral functions $A(\omega)\big|_n$, given by Eq.(31), plotted for $n = 4, 5, 6, 7$, where the poles have been removed by convolution with L_δ given in Eq.(34), where delta is given for each of these curves in the title as $\delta = 0.27$, again all measured in units of the bandwidth. It is chosen as the smallest constant such that there are no peaks visible even for the last iteration. As in Figure 2, the convergence is obscure, resulting from the short chains. We see also that in this method, were the broadening is not adapted to the chain length, the approximated spectral function chane slower from one iteration to another, although it is not clear whether this is a disadvantage.

6 Pertubative Treatment Of The Bath

In the chapter before, we faced some problems connected to the question how to obtain a smooth function out of a discrete set of eigenenergies. In this section, we will - following again Anders - try to give an answer.

Our strategy will be to not cut off the last bath, for it is responsible for the broadening. Since we cannot solve the system exactly, this was the assumption, we will instead employ an approximation for the influence of the bath on the chain. This turns out to suffice for a physical broadening of the spectral function. The justification for the approximation is the very reason we regarded a chain instead of the initial Hamiltonian: we assumed that the relevant behaviour is already captured in the chain, so that the influence of the reservoir is small and can be treated as a pertubation. In Section 3.2 we used exactly this approximation scheme to obtain an expression for the Green's Function in Eq.(16). In this section, we will make this more general to incorporate higher correlators.

6.1 A Basis In Green's Function Space

Assume we have a chain of length n, whose Hamiltonian was diagonalized simultaneously with the number operator

$$N^{chain} = \sum_{k=-1}^{n} \sum_{\nu} n_{k\nu},$$

and the chain spin operator

$$S^{chain} = \sum_{k=-1}^{n} \sum_{\nu} \nu \; n_{k\nu},$$

with eigenvalues $\{E_k\}$, $\{N_k\}$, $\{s_k\}$ and eigenvectors $\{|N, s, E\rangle\}$. N labeling the subspace with N particles, s the label for the subspace with spin s and E a index to lift the remaining degeneracy. This will only be important later, so for now exchange the two labels by just one, say r, indexing all states.

Then the Hamiltonian can be written in terms of the Hubbard-Operators

$$X_{rs} = |r\rangle \otimes \langle s|,$$

where it is understood that these operators act trivially on the bath Fock space. As a result, the diagonal operators X_{rr} form a set of projection operators which sum up to the identity, as we used before.

In the following we will choose our eigenvectors and operators such that the matrix elements $(f_{n\nu})_{kl} = Tr\{X_{lk}f_{n\nu}\}$ are real[6]. To see how to write the Hamiltonian in terms of these opera-

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[6]This can be done, since as we saw in Section 5.3, we can choose the Hamiltonian to be real symmetric, thus having a orthonormal set of real eigenvectors.

tors, we compute:

$$H^I = t_n \sum_\nu b_{n\nu}^\dagger \left(\sum_k X_{kk} \right) f_{n\nu} \left(\sum_l X_{ll} \right) + t_n \left(\sum_l X_{ll} \right) f_{n\nu}^\dagger \left(\sum_l X_{kl} \right) b_{n\nu} =$$

$$= \sum_{(kl);\nu} \left(t_n b_{n\nu}^\dagger X_{kl} (f_{n\nu})_{kl} + t_n X_{lk} (f_{n\nu}^\dagger)_{lk} b_{n\nu} \right) =$$

$$= \sum_{(kl);\nu} t_n (f_{n\nu})_{kl} \left(b_{n\nu}^\dagger X_{kl} - b_{n\nu} X_{lk} \right).$$

Note the minus sign in the 3rd line which we obtained by anticommuting the fermionic operators b and X. Their equal-time-anticommutators are equal to 0, due to the fact that X and b act nontrivially only one the chain respectively the reservoir.
Our Hamiltonian reads:

$$H = \sum_a E_a X_{aa} + \sum_{\mathbf{k}\nu} \epsilon_{\mathbf{k}} b_{\mathbf{k}n\nu}^\dagger b_{\mathbf{k}n\nu} + \sum_{(kl);\nu} t_n (f_{n\nu})_{kl} \left(b_{n\nu}^\dagger X_{kl} - b_{n\nu} X_{lk} \right)$$

$$b_{n\nu}^\dagger = \sum_{\mathbf{k}} \lambda_{\mathbf{k}n\nu} b_{\mathbf{k}n\nu}^\dagger,$$

and we calculate equal-time (anti-)commutators:

$$[X_{kl}, X_{rs}] = \delta_{lr} X_{ks} - \delta_{sk} X_{rl}$$

$$\{X_{kl}, X_{rs}\} = \delta_{lr} X_{ks} + \delta_{sk} X_{rl}$$

$$[b_{n\nu} X_{kl}, X_{rs}] = b_{n\nu} X_{kl} X_{rs} - X_{rs} b_{n\nu} X_{kl} = b_{n\nu} (X_{kl} X_{rs} + X_{rs} X_{kl})$$

$$= b_{n\nu} \{X_{kl}, X_{rs}\}$$

$$[H, X_{rs}] = t_n \sum_{(kl);\nu} (f_{n\nu})_{kl} \left(b_{n\nu}^\dagger (\delta_{lr} X_{ks} + \delta_{sk} X_{rl}) - b_{n\nu} (\delta_{kr} X_{ls} + \delta_{sl} X_{rk}) \right) +$$

$$+ (E_r - E_s) X_{rs}$$

$$[H, b_{\mathbf{q}n\nu}] = -t_n \sum_{kl} \lambda_{\mathbf{q}n} (f_{n\nu})_{kl} X_{kl} - \epsilon_{\mathbf{q}} b_{\mathbf{q}n\nu}$$

$$[H, b_{\mathbf{q}n\nu}^\dagger] = t_n \sum_{kl} \lambda_{\mathbf{q}n}^* (f_{n\nu})_{kl} X_{lk} + \epsilon_{\mathbf{q}} b_{\mathbf{q}n\nu}^\dagger.$$

With these preparations, the E.O.M. method for

$$\mathcal{G}_{X_{rs}, X_{uv}}^R (t - t') = -i\theta(t - t') \langle \{X_{rs}(t), X_{uv}(t')\} \rangle_T$$

will lead us together with some approximations to an equation for the Green's Functions of the System. Note that here we want to insert the full dynamics, not only of the chain, whereas our eigenstates - from which we builded the Hubbard operators - are only eigenstates of the chain dynamics.
After the definition of

$$W_{(rs)(uv)} = \langle \{X_{rs}, X_{uv}\} \rangle_T = \delta_{su} \langle X_{rv} \rangle_T + \delta_{rv} \langle X_{us} \rangle_T$$

we deduce the equation of motion

$$[\omega + (E_r - E_s)]\mathcal{G}^R_{X_{rs},X_{uv}}(\omega) = W_{(rs)(uv)}+$$
$$+ t_n \sum_{(kl);\nu} (f_n)_{kl} \left((\delta_{lr}\mathcal{G}^R_{b^\dagger_{n\nu}X_{ks},X_{uv}} + \delta_{sk}\mathcal{G}^R_{b^\dagger_{n\nu}X_{rl},X_{uv}}) - (\delta_{kr}\mathcal{G}^R_{b_{n\nu}X_{ls},X_{uv}} + \delta_{sl}\mathcal{G}^R_{b_{n\nu}X_{rk},X_{uv}}) \right),$$

where we already differentiated in time and expanded in Fourier modes.

In principle, one could search for other equations of motions for the other involved Green's functions, but this would not yield a closed set of equations, since in the general case $U \neq 0$, we will generate higher and higher polynomials of operators. So instead, we directly perform a mean-field like approximation, also known as Hubbard I approximation[7]

$$\mathcal{G}^R_{b_n X_{ks},X_{uv}} \approx -\langle X_{rs}\rangle_T\ \mathcal{G}^R_{b_n,X_{uv}} \tag{36}$$

It is worthwile to contemplate this approximation. A priori, the coupling between reservoir and impurity is not necessarily weak - it is a system parameter and can be chosen arbitrary. However, by mapping the system on a chain, we will include higher and higher correlations, since by each iteration former correlations between chain and bath are then captured by correlators between chain operators, whose hierarchy remains untruncated.

We need to evaluate averages of the form $\langle X_{rs}\rangle_T$. To do so, we would need the eigenvectors and eigenenergies of the full Hamiltonian, which we do not have; however, we assumed that the main physics should already be contained in the chain Hamiltonian, with the additional reservoir only giving small corrections - which can be treated pertubatively - this motivates the approximated density matrix

$$\rho_\beta\big|_n = \frac{e^{-\beta H^{approx}_n}}{Tr\{e^{-\beta H^{approx}_n}\}} = \sum_k \frac{e^{-\beta E_k}}{Z} X_{kk},$$

where Z is the partition function and H^{approx}_n is given by Eq.(29), and the corresponding approximation of the true thermal average with the chain average

$$\langle X_{rs}\rangle_T \approx \sum_k \frac{e^{-\beta E_s}}{Z} Tr\{X_{kk}X_{rs}\} = \delta_{rs}\frac{e^{-\beta E_s}}{Z} \overset{\beta \to \infty}{\to} \frac{1}{\sharp} \sum_{\alpha \in GS} \delta_{r\alpha}\delta_{s\alpha}, \tag{37}$$

Here "$\sharp$" should denote the degeneracy of the ground state of the chain Hamiltonian Eq.(29), and the sum is over its subspace. With Eq.(36), we obtain

$$[\omega + (E_r - E_s)]\mathcal{G}^R_{X_{rs},X_{uv}}(\omega) = W_{(rs)(uv)}+$$
$$- t_n \sum_{(kl);\nu} (f_{n\nu})_{kl} \left((\delta_{lr}\langle X_{ks}\rangle_T + \delta_{sk}\langle X_{rl}\rangle_T)\mathcal{G}^R_{b^\dagger_{n\nu},X_{uv}}+ \right.$$
$$- (\delta_{kr}\langle X_{ls}\rangle_T + \delta_{sl}\langle X_{rk}\rangle_T)\mathcal{G}^R_{b_{n\nu},X_{uv}} \Big) =$$
$$= W_{(rs)(uv)} - t_n \sum_{(kl);\nu;\mathbf{q}} (f_{n\nu})_{kl} \left(W_{(kl)(rs)}\lambda^*_{\mathbf{q}n}\mathcal{G}^R_{b^\dagger_{\mathbf{q}n\nu},X_{uv}} - W_{(lk)(rs)}\lambda_{\mathbf{q}n}\mathcal{G}^R_{b_{\mathbf{q}n\nu},X_{uv}} \right).$$

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[7]Since X_{kl} is a fermionic operator, its expectation value will be an anticommuting or Grassmann number.

Later, we will be interested in the impurity Green's function, where the operator X_{uv} in $\mathcal{G}^R_{b^\dagger_{\mathbf{q}n\nu}, X_{uv}}$ will be an creation operator[8]. We know that the total particle number of chain and bath is conserved and thus an expectation value like $\langle A \rangle_T$, where A changes the number of particles, will be zero. It follows that $\mathcal{G}^R_{b^\dagger_{\mathbf{q}n\nu}, X_{uv}} = 0$ if X_{uv} is a creation operator. For now, to not stretch the meaning of the word "equation" any further, we will keep this term nontheless. We close now to a system of equations by using the previously calculated commutators:

$$(\omega - \epsilon_{\mathbf{q}})\mathcal{G}^R_{b_{\mathbf{q}n\nu}, X_{uv}}(\omega) = t_n \sum_{(kl)} \lambda_{\mathbf{q}n}(f_{n\nu})_{kl}\mathcal{G}^R_{X_{kl}, X_{uv}}(\omega)$$

$$(\omega + \epsilon_{\mathbf{q}})\mathcal{G}^R_{b^\dagger_{\mathbf{q}n\nu}, X_{uv}}(\omega) = -t_n \sum_{(kl)} \lambda^*_{\mathbf{q}n}(f_{n\nu})_{kl}\mathcal{G}^R_{X_{lk}, X_{uv}}(\omega).$$

Now use:

$$\Sigma_n(\omega) := |t_n|^2 \sum_{\mathbf{q}} \frac{|\lambda_{\mathbf{q}n}|^2}{\omega - \epsilon_{\mathbf{q}}}.$$

Define

$$E_{(rs)(xy)} = (E_s - E_r)\delta_{(rs)(xy)},$$

Where $\delta_{(rs)(xy)} = \delta_{rx}\delta_{sy}$ and

$$\Sigma_{(rs)(ab)} = -\sum_{(kl);\nu} (f_{n\nu})_{kl} \left(W_{(kl)(rs)}\Sigma_n(-\omega)(f_{n\nu})_{ba} - W_{(lk)(rs)}\Sigma_n(\omega)(f_{n\nu})_{ab} \right)$$

as well as

$$G_{(xy)(uv)}(\omega) := \mathcal{G}^R_{X_{xy}, X_{uv}}(\omega).$$

The equation of motion thus has the form:

$$\sum_{xy} [\omega\delta_{(rs)(xy)} - E_{(rs)(xy)} - \Sigma_{(rs)(xy)}]G_{(xy)(uv)}(\omega) = W_{(rs)(uv)}.$$

To make the formula more transparent and in order to use usual matrix notation, consider for chain length n:

$$\mathbb{N}^2 \overset{\phi}{\mapsto} \mathbb{N}, \quad (r, s) \mapsto d^n(r-1) + s.$$

Where d is the size of the Hilbert space one started with, in our case of spin-$\frac{1}{2}$-fermions, $d = 4$. note that e.g the set $([1, 4] \times [1, 4]) \cap \mathbb{N}^2$ is mapped to $[1, 16] \cap \mathbb{N}$, so we can reformulate the above equation in classical vector-matrix-notation:

$$[\omega\mathbf{1} - \mathbf{E} - \mathbf{\Sigma}(\omega)]\vec{G}_\beta(\omega) = \vec{W}_\beta, \tag{38}$$

where the vector $\vec{G}_\beta$ has the elements $(\vec{G}_\beta)_\alpha = G_{\psi(\alpha),\psi(\beta)}$ and

$$\mathbb{N} \overset{\psi}{\mapsto} \mathbb{N}^2, \quad \alpha \mapsto \left(\left\lceil \frac{\alpha}{d^n} \right\rceil, (\alpha - 1) \mod d^n + 1 \right),$$

---

[8]More to this later in Section 6.2. The question is not important at this point.

with $\lceil \cdot \rceil$ the Gauss bracket, returning the smallest integer bigger than its argument.
to simplify the expressions for the other involved matrices, we introduce a permutation matrix
$\mathbf{P}$

$$\mathbb{R}^{d^{2n}} \overset{\mathbf{P}}{\mapsto} \mathbb{R}^{d^{2n}}, \quad \vec{v} \mapsto \mathbf{P}\vec{v};$$

$$\mathbf{P}\vec{e}_{\phi(r,s)} = \vec{e}_{\phi(s,r)},$$

where $\{\vec{e}_\alpha\}$ denotes a basis.
Then:

$$\boldsymbol{\Sigma}(\omega) = \sum_\nu \Sigma_n(\omega)\vec{f}_{n\nu} \otimes \vec{f}_{n\nu} \cdot \mathbf{PW} - \sum_\nu \Sigma_n(-\omega)\mathbf{P}\vec{f}_{n\nu} \otimes \vec{f}_{n\nu} \cdot \mathbf{W} \tag{39}$$

where $\vec{f}_{n\nu}$ is the vector with elements $(\vec{f}_{n\nu})_{\phi(r,s)} = (f_{n\nu})_{rs}$.

6.2 Representation Of Other Green's Functions In This Base

Given $G_{(xy)(uv)}(\omega)$, we can obtain the expression for $\mathcal{G}^R_{f_{-1\nu}, f^\dagger_{-1\nu}}$ by the following procedure: We have constructed the Hubbard operators $\{X_{kr}(t)\}_{kr}$ such that they form a partition of unity at each time t, therefore

$$\{f_{-1\nu}(t), f^\dagger_{-1\nu}(t')\} =$$

$$= \left\{ \left(\sum_k X_{kk}(t) \right) f_{-1\nu}(t) \left(\sum_l X_{ll}(t) \right), \left(\sum_j X_{jj}(t') \right) f^\dagger_{-1\nu}(t') \left(\sum_i X_{ii}(t') \right) \right\} =$$

$$= \sum_{klji} (f_{-1\nu})_{kl}(f_{-1\nu})_{ij}\{X_{kl}(t), X_{ji}(t')\}$$

must hold. Remarkably there is no time dependency of $(f_{-1\nu})_{kl}$ since

$$X_{kk}(t)f_{-1\nu}(t)X_{ll}(t) = e^{iHt}X_{kk}e^{-iHt}e^{iHt}f_{-1\nu}e^{-iHt}e^{iHt}X_{ll}e^{-iHt} = e^{iHt}X_{kk}f_{-1\nu}X_{ll}e^{-iHt}.$$

So the impurity Green's function is given by

$$\mathcal{G}^R_{f_{-1\nu}, f^\dagger_{-1\nu}}(\omega) = \sum_{klji} (f_{-1\nu})_{kl}(f_{-1\nu})_{ij}G_{(kl)(ji)}(\omega),$$

which reads in our matrix-vector-notation:

$$\mathcal{G}^R_{f_{-1\nu}, f^\dagger_{-1\nu}}(\omega) = \vec{f}_{-1\nu} \cdot \mathbf{G}(\omega)\mathbf{P}\vec{f}_{-1\nu},$$

where again the notation $(\vec{f}_{-1\nu})_\alpha = (f_{-1\nu})_{\psi(\alpha)}$ was used.

At this point we want to exploit our symmetries, therefore we change back to our notation $|N, s, E\rangle$ for the eigenstates. A general chain operator A can be written as:

$$A = \sum_{NsE;N's'E'} A^{N,s,E}_{N',s',E'}|N, s, E\rangle\langle N', s', E'|.$$

Now assume that we are not interested in just any operator, but one that changes between the N- and the s-subspaces in a controlled way, so we request:

$$N - N' = \Delta N, \quad s - s' = \Delta s,$$

where ΔN and Δs are numbers that we fix in advance. An operator with these operators, say B, we can thus write as

$$B = \sum_{NsEE'} B^{N,s,E}_{N-\Delta N, s-\Delta s, E'} |N, s, E\rangle \langle N - \Delta N, s - \Delta s, E'|.$$

When B falls into such a restricted class of operators, then $[H, B]$ will do as well. Indeed:

$$[H, A] = \sum_{NsEE';MtF} B^{N,s,E}_{N-\Delta N, s-\Delta s, E'} H_{M,t,F} \left[|M, t, F\rangle\langle M, t, F|N, s, E\rangle\langle N - \Delta N, s - \Delta s, E'| + \right.$$

$$- |N, s, E\rangle\langle N - \Delta N, s - \Delta s, E'|M, t, F\rangle\langle M, t, F| \big] =$$

$$= \sum_{NsEE';MtF} B^{N,s,E}_{N-\Delta N, s-\Delta s, E'} H_{M,t,F} \left[|M, t, F\rangle\langle N - \Delta N, s - \Delta s, E'|\delta_{MN}\delta_{ts}\delta_{FE} + \right.$$

$$- |N, s, E\rangle\langle M, t, F|\delta_{N-\Delta N, M}\delta_{s-\Delta s, t}\delta_{E'F} \big] =$$

$$= \sum_{NsEE'} B^{N,s,E}_{N-\Delta N, s-\Delta s, E'} (H_{N,s,E} - H_{N-\Delta N, s-\Delta s, E'}) |N, s, E\rangle\langle N - \Delta N, s - \Delta s, E'|.$$

By this basic linear algebra manipulation, we can now severely restrict the space in which we diagonalize our matrix. Define therefore for $a, b \in \mathbb{Z}$:

$$\kappa_{a,b} = \left\{ A \in \mathcal{B}(\mathcal{H}^{chain}) \big| \ \Delta N(A) = a, \ 2\Delta s(A) = b \right\},$$

with $\mathcal{B}(\mathcal{H}^{chain})$ the set of operators on the chain; in particular the $\{X_\alpha\}$ form a basis of this space. The notation $\Delta N(A)$ shall denote that the operator A falls precisely in such a above mentioned class, it is not a function[9] of A. More adapted to our question, define

$$\kappa_+ = \kappa_{1,1}, \quad \kappa_- = \kappa_{-1,-1}.$$

The choices of the signs reflect our choices about which operators we are interested in; here this choice will lead to the $(f_{-1\uparrow}, f^\dagger_{-1\uparrow})_\omega$ Green's function. We denoted the relevant subspaces for the Green's function we are interested in by a shorthand notation for convenience. For other spins definitions are analogous; we know now that our chain Hilbert space decomposes as direct sum of these smaller spaces:

$$\mathcal{H}^{chain} = \bigoplus_{(a,b)\in\mathbb{Z}^2} \kappa_{a,b},$$

Finally, we want Green's functions with the first entry from κ_-, hence a $\uparrow$-annihilation operator, and the second from κ_+, hence a $\uparrow$-creation operator. Thus, we modify equation Eq.(38) by

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[9]this would not be defined for a general operator A, although it is for our basis $\{X_\alpha\}$.

only considering a subspace in the following way: the vector index of $\vec{G}_\beta$ should be from κ_-, while the index β should be from κ_+. Thus, The Matrix $[\omega\mathbf{1} - \mathbf{E} - \boldsymbol{\Sigma}(\omega)]$ only acts in κ_-, while the family of vectors $\vec{W}_\beta$ is of the same type as $\vec{G}_\beta$. We write this schematically:

$$[\omega\mathbf{1} - \mathbf{E} - \boldsymbol{\Sigma}(\omega)]_{\kappa_-\kappa_-}\mathbf{G}_{\kappa_-\kappa_+}(\omega) = \mathbf{W}_{\kappa_-\kappa_+}.$$

Furthermore, since we are finally only interested in $\mathcal{G}^R_{f_{-1\nu},f^\dagger_{-1\nu}}$, we can reduce numerical effort further by contracting the second index of $\mathbf{G}$ with $\mathbf{P}\vec{f}_{-1\nu}$, since it does not participate in the inversion process:

$$[\omega\mathbf{1} - \mathbf{E} - \boldsymbol{\Sigma}(\omega)]_{\kappa_-\kappa_-}\vec{G}_\omega = \vec{W} \tag{40}$$

$$\vec{W}_\nu := \mathbf{W}_{\nu\kappa_-\kappa_+}(\mathbf{P}\vec{f}_{-1\nu})_{\kappa_+} \quad \vec{G}_\omega := \mathbf{G}_{\nu\kappa_-\kappa_+}(\omega)(\mathbf{P}\vec{f}_{-1\nu})_{\kappa_+}. \tag{41}$$

This results in the same outcome, but with decreased numerical effort. For illustration, some numbers will be given in the following table:

n	D	d
-1	16	2
0	256	24
1	4096	300
2	65536	3920

with $D = \dim(\mathcal{H}^{chain} \otimes \mathcal{H}^{chain})$, $d = \dim(\kappa_+)$ and n the chain length. This seems to be growing exponentially as well.

6.3 Numerical Implementation

In this Section some numerical results related to Eq.(40) shall be discussed. In all plots, we will be interested in the approximated spectral function

$$\mathcal{G}^R_{f_{-1\nu},f^\dagger_{-1\mu}}(\omega)\big|_n = \vec{f}_{-1\mu} \cdot \vec{G}^{(n)}_{\nu\omega} \tag{42}$$

$$A(\omega)\big|_n = \Im\mathcal{G}^R_{f_{-1\nu},f^\dagger_{-1\mu}}(\omega)\big|_n \tag{43}$$

where the superscript (n) denotes that here the chain Hamiltonian H^{approx}_n given in (Eq.29) was used in obtaining $\vec{G}^{(n)}_{\nu\omega}$.

We start by solving Eq.(40) for $n = -1$ and $U \neq 0$, where some analytic solutions were obtained in Section 3.2 whose comparison to the program is plotted in Figure 4. We compare here the imaginary parts of Eq.(42) and Eq.(16), and In these plots we see that the resulting spectral function depends heavily on the degeneracy of the ground state of the chain, as we could have guessed from Section 3.2.

We can see how this influences the spectral functions from longer chains in Figure 5, as the even-odd-behaviour is quiet different depending on the ground state degeneracy of the chain.

Another Check of the program is obtained by setting t_{-1} close to zero; in this limit, where the hopping term $\propto t_{-1}$ vanishes, we get a discrete level system which is actually represented by

Eq.(31). This one can see for $n = 0$, as in Figure 6 in the bottom plot. The three spikes are reminiscences of the three delta-functions centered roughly at 0, ϵ_{-1} (twofold degenerate) and $\epsilon_{-1}+U$. There is some disagreement, since for finite t_{-1}, not only the delta peaks get reglarized, but also the two levels symmetric around zero get pushed outwards by the hybridization to the bath, as can be seen in the other two plots in the same figure.

Furthermore, we can ask what happens if we have no interaction, i.e. $U = 0$. In this case the here described approximation scheme is exact, since in the equations of motion for the impurity Green's function only Green's function with one-particle operators appear, thus Eq.(36) is an identity. That this is indeed the case, one can see in Figure 7, where the approximate impurity spectral function is plotted for different chain lengths and $U = 0$.
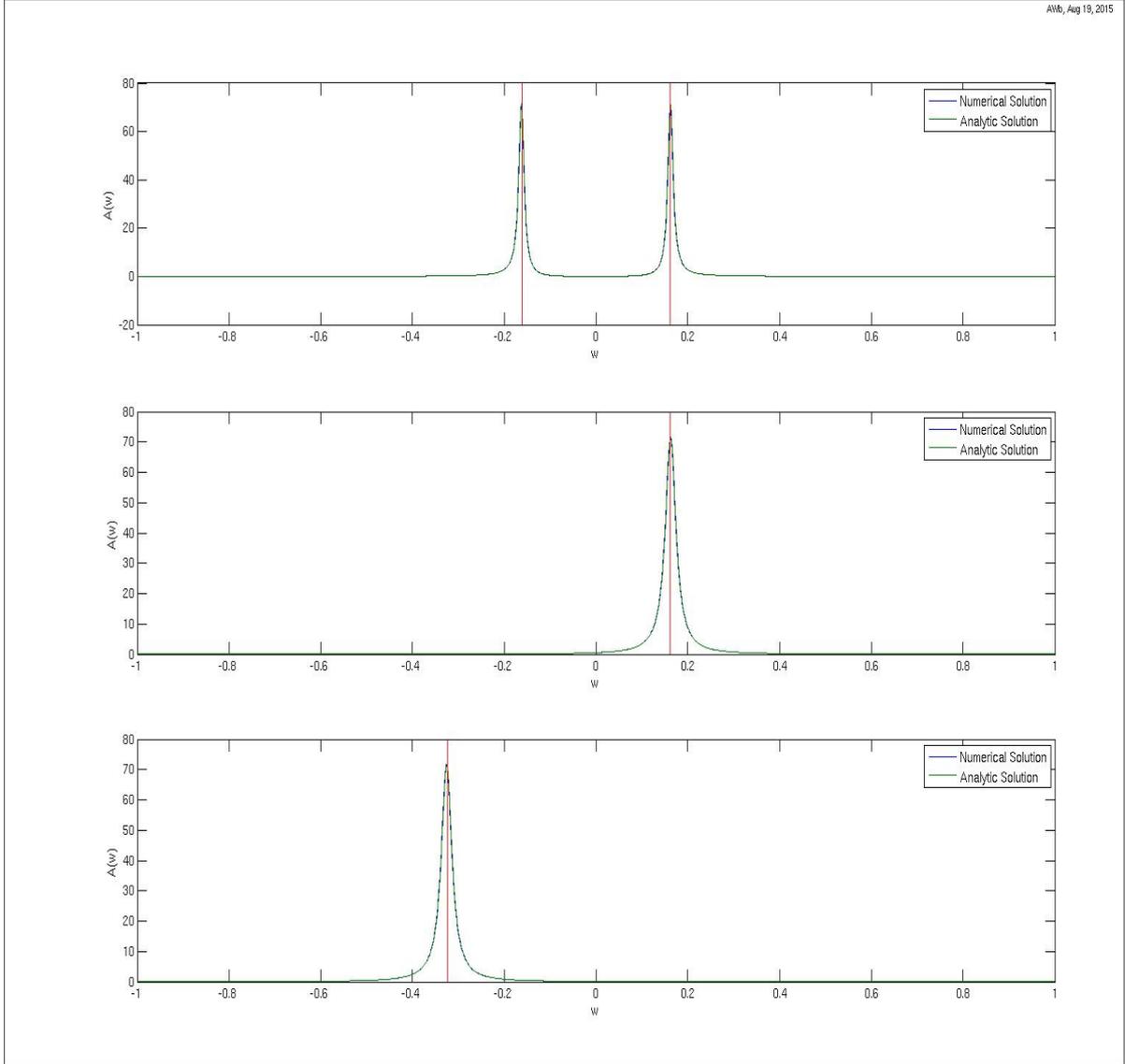
Figure 4: The impurity spectral function is plotted for $n = -1$, $U = 0.324$, $\epsilon_{-1} \in \{-\frac{U}{2}, \frac{U}{2}, -2U\}$ in the three pictures from top to bottom picture respectively and $t^2_{-1} = 0.02793$ against the frequency ω, which is linearly discretized with spacing 0.0005. Energies are measured in units of the bandwidth and the initial bath spectral function is given by Eq.(33). The curve labeled "Numerical Solution" is the one obtained by combination of Eq.(40) and Eq.(42) and taking the imaginary part $A(\omega)\big|_n$, while the other one is given by Eq.(16), again by taking the imaginary part. Not surprisingly in each plot we can identify only one curve although there are two labels: this is because both functions were obtained by the same steps and approxmations. But we can see something interesting going on: for $\epsilon_{-1} = -\frac{U}{2}$, we have a twofold degenerate ground state, which results in two distinct peaks at ϵ_{-1} and $\epsilon_{-1} + U$ - indicated by red lines - while for $\epsilon_{-1} = \frac{U}{2}$ the ground state is unique and we have just one peak at position $\epsilon_{-1} = \frac{U}{2}$ - we see here the interaction has no influence since the ground state is empty and thus experiences no interaction effects. Now for the last plot: here the ground state is the fully occupied state, thus it experiences the interaction and the peak is at position $\epsilon_{-1} + U = -U$.
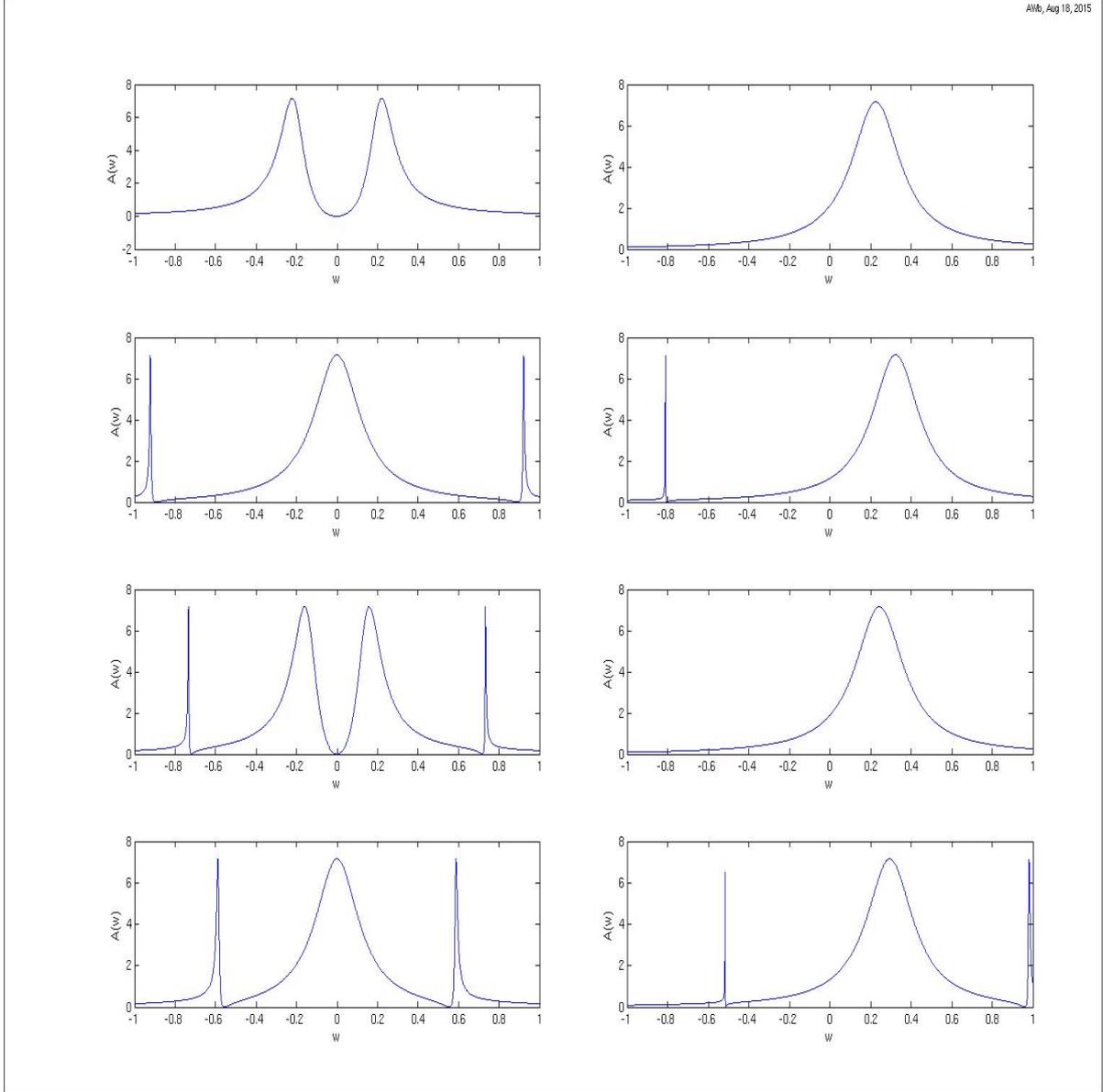
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Figure 5: The impurity spectral function $A(\omega)\big|_n$ given by Eq. (43) is plotted agains the frequency ω with linear discretization 0.0005, where all energies are measured in units of the bandwidth. In all plots, $U = 0.4324$ and $t_{-1}^2 = 0.2793$. $\epsilon_{-1} = \mp\frac{U}{2}$ on the left respectively the right side, and from $n = -1$ for the plots at the top to $n = 2$ for the plots at the bottom. For $\epsilon_{-1} = -\frac{U}{2}$, the spectral function is symmetric and has an even-odd characteristic behaviour, resulting from the fact that for odd chain lengths the chain ground state is not unique. If $\epsilon_{-1} = \frac{U}{2}$ this is absent. The main peak keeps its asymmetric shape, but is slightly moved around.
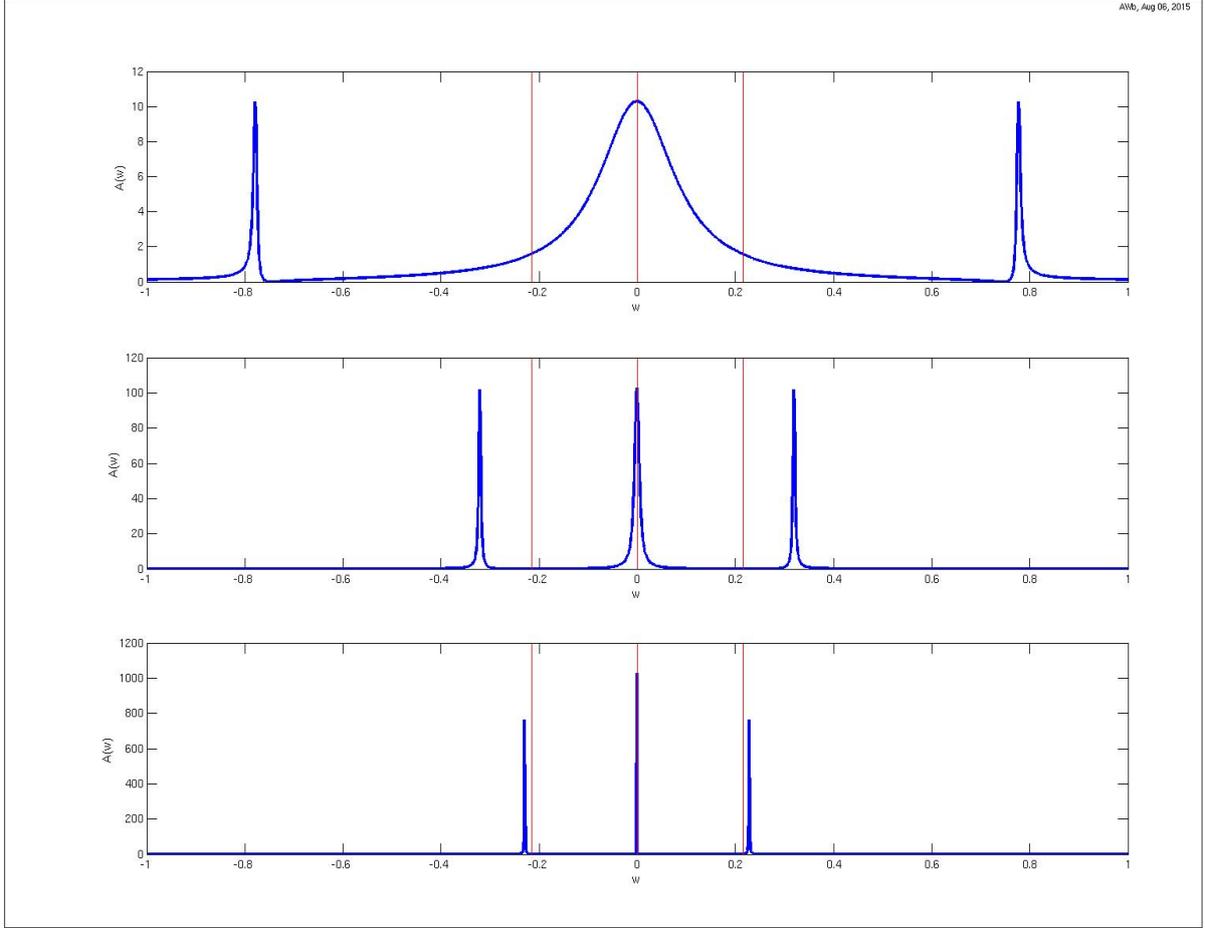
Figure 6: The impurity spectral function $A(\omega)\big|_n$ is plotted as the blue, thick curve for $n = 0$, $U = 0.4324$, $\epsilon_{-1} = -\frac{U}{2}$ and $t_{-1}^2 \in \{0.1943, 0.01943, 0.001943\}$, respectively from above to below against the frequency ω linearly discretized with spacing 0.001. Energies are measured in units of the bandwidth and the initial bath spectral function is given by Eq.(33). The red vertical lines are obtained by the eigenenergies of the impurity hamiltonian Eq.(3): they correspond to the energy differences of the eigenenergies to the ground state, as in the Lehmann representation. Here one sees that increasing the hybridization t_{-1}^2, the two nonzero energylevels are repelled by each other and thus the distance of these two energy levels increases.
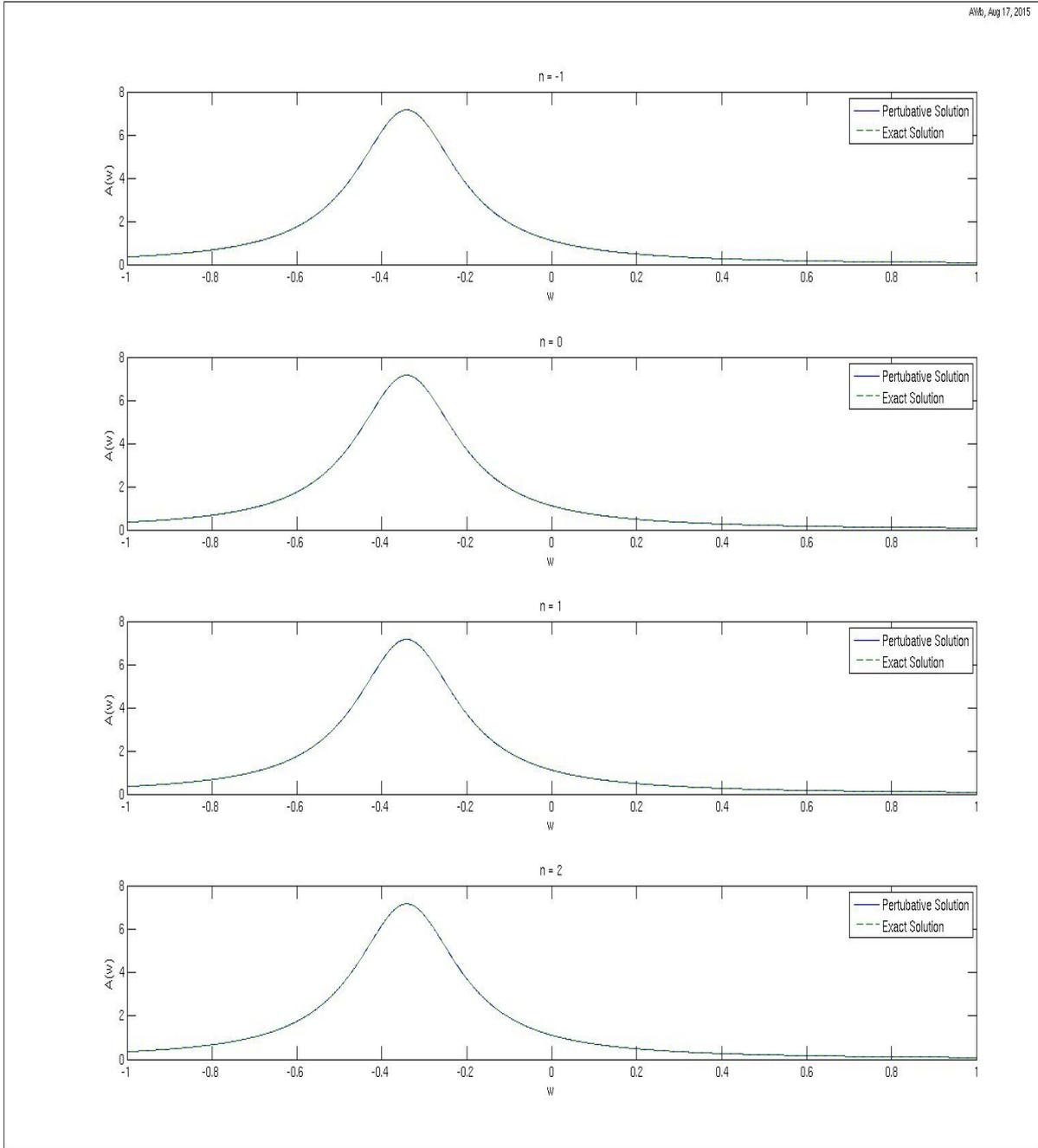
Figure 7: The impurity spectral function is plotted for $U = 0.4324$, $\epsilon_{-1} = -0.3252$, $t_{-1}^2 = 0.2793$ and $n \in \{-1, 0, 1, 2\}$, respectively from top to bottom, against the frequency ω, which is linearly discretized with spacing 0.0005. Energies are measured in units of the bandwidth and the initial bath spectral function is given by Eq.(33). The curve labeled "Numerical Solution" is the one obtained by combination of Eq.(40) and Eq.(42) and taking the imaginary part $A(\omega)\big|_n$, while the other one with the label "Exact Solution is given by inserting Eq.(28) into Eq.(13). As on can see, in fact there is only one curve because the two agree. This means the approximation Eq.(37) is exact in this case.

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References

[1] F.B.Anders, to be published

Selbstständigkeitserklärung

Hiermit versichere ich, dass ich diese Bachelorarbeit zum Thema ,,Verbreiterung von Spektral-Funktionen des diskretisierten Single Impurity Anderson Model" selbstständig verfasst habe. Ich habe keine anderen als die angegebenen Quellen und Hilfsmittel benutzt, sowie Zitate kenntlich gemacht.

Mir ist bekannt, dass Zuwiderhandlung auch nachträglich zur Aberkennung des Abschlusses führen kann.

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