Towards a solution of the CTMA integral equations and its implications for the dynamics of strongly correlated electron systems.

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Plan of talk.

- Warm up: Some of the material was presented at Hvar 2002, at Ustron 2004, and at Dresden 2005.
- Ultimate goal: Treat the strongly correlated Anderson- or Kondo-lattice with DMFT and its generalizations. Needed is an impurity solver (Anderson impurity model.
- Present state of the DMFT: Advantages and drawbacks.
- Why is a parquet approach needed?
- First results.

Warm-up: Resolvent perturbation technique.

Express partition- and Green's functions in terms of resolvents $(z - \hat{H}_0 - \hat{V})^{-1}$ and expand in the *hybridization* $\hat{V}$:

$$\mathcal{Z} = Tre^{-\beta\hat{H}} = \frac{1}{2\pi i}\oint dz e^{-\beta z} Tr(z - \hat{H}_0 - \hat{V})^{-1}$$

(Contour counter-clockwise). Trace out the band electrons and write explicitly Tr_f as a sum on the empty f-level and the occupied one. Double occupation is forbidden for the $U \to \infty$. Hamiltonian:

$$\hat{H} = \sum_\sigma (\epsilon_f f^\dagger_\sigma f_\sigma + \sum_k (\epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + [V f^\dagger_\sigma c_{k\sigma} + h.c] f_{-\sigma} f^\dagger_{-\sigma}))$$

$$\mathcal{Z} = \mathcal{Z}_{band}\mathcal{Z}_f = \mathcal{Z}_{band}\oint \frac{dz}{2\pi i} e^{-\beta z}(P_0(z) + \sum_\sigma P_\sigma(z))$$

The auxiliary propagators P are related to their self-energies Σ.

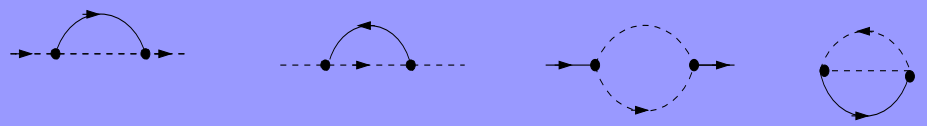
$$P_0(z-\epsilon_k) = \frac{1}{z-\epsilon_k-\Sigma_0(z-\epsilon_k)} \; ; P_\sigma(z+\omega) = \frac{1}{z+\omega-\epsilon_f-\Sigma_\sigma(z+\omega)}$$

The simplest (self consistent) expressions for the self-energies are

$$\Sigma_0(z) = \sum_{k\sigma} V^2 f(\epsilon_k) P_\sigma(z+\epsilon_k) \rightarrow \sum_\sigma \int d\omega V^2 f(\omega) N(\omega) P_\sigma(z+\omega)$$

$$\Sigma_\sigma(z) = \int d\omega V^2 (1-f(\omega)) N(\omega) P_0(z+\omega)$$

($N(\omega)f(\omega) = DOS\times$ Fermi's function). This system of eqs. is called NCA and was set up by H.K. and J.Kimball (1970). Visualized by diagrams:



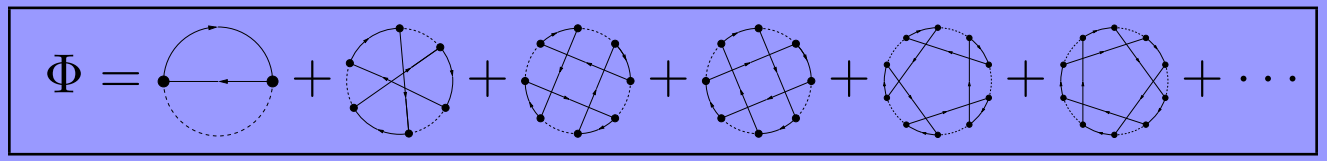
The diagrams are the self energies in the empty and the filled f-level, the contribution to Green's function for the f-electrons,

$$\mathcal{Z}_f \mathcal{G}_f(i\omega_n) = \oint \frac{dz}{2\pi i} P_0(z) P_\sigma(i\omega_n + z)$$

and the generating functional of the NCA (Kuramoto 1970). $i\omega_n$ are the usual Matsubara frequencies for electrons, and $V^2\mathcal{G}_f(i\omega_n)$ enters into the DMFT-loop.
Two disadvantages of the NCA have turned out:
1.) The threshold behavior of the auxiliary propagators is incorrect: the exponents do not depend on the occupation of the f-level.
2.) In the Schrieffer-Wolff limit, where the s-f model and an *additional normal potential* is obtained, the normal potential part is treated insufficiently within the NCA.
This ends the warm-up.

The Consistent t-matrix approximation

(CTMA) [J.Kroha, P. Wölfle, T.A.Costi, Phys. Rev. Letters **79**, 261 (1997)] was set up to avoid the disadvantages of the NCA. It starts from a generating functional, in which the f-level is represented as the periphery of a circle with alternating occupation.



The straight lines for the band electrons cross only two vertices on the circle. Near the axis of the wheels the band electrons generate a direction of rotation: clockwise and counter-clockwise. Up to the 8th order the procedure is exact, from 10th and higher orders on only one clockwise and one counter-clockwise diagram is taken into account.

The self energies are obtained by cutting the dashed lines on the wheel periphery. They can be related to scattering matrix-equations with three energy variables: the total energy entering (1st), leaving (2nd) and running through all intermediate states (3rd) of the corresponding diagrams. For $\Sigma_0(z)$ the following scattering matrix is needed:

$$\begin{aligned} & T^0(z+\omega_1, z+\omega_2, z) + V^2 P_\sigma(z+\omega_1+\omega_2) \\ = & -\int d\omega T^0(z+\omega, z+\omega_2, z) I^0(z+\omega_1, z+\omega, z), \end{aligned}$$

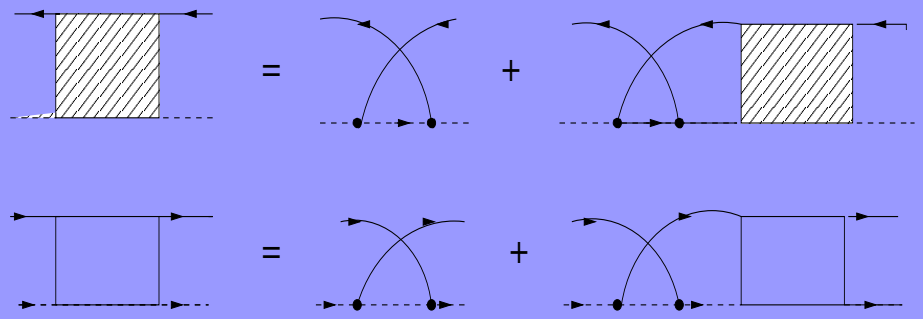
similarly, for $\Sigma_\sigma(z)$, the scattering matrices, in which for symmetry reasons the total energy $z-(-\omega_1)$ enters into the diagrams

$$\begin{aligned} & T^\pm(z+\omega_1, z+\omega_2, z) \pm V^2 P_0(z+\omega_1+\omega_2) \\ = & -\int d\omega T^\pm(z+\omega, z+\omega_2, z) I^\pm(z+\omega_1, z+\omega, z) \end{aligned}$$

In the CTMA the kernels (with the intermediate propagators) read:

$$
\begin{aligned}
I^0(\cdots) &= V^2 N(\omega) f(\omega) P_0(z+\omega) P_\sigma(z+\omega+\omega_1) \\
I^{\pm}(\cdots) &= V^2 N(-\omega) f(\omega) P_\sigma(z+\omega) P_0(z+\omega+\omega_1)
\end{aligned}
$$

reflecting *uncoupled Bethe-Salpeter equations*.



1.) These can be turned into nonlinear integral equations by Sudakov's trick (see Nozières et al., Phys. Rev. **178** 1085 (1969)):

Iterating the eqs., one rewrites the integrals as follows

$$\int d\omega_3 \int d\omega_4 = \int d\omega_3 \int^{\omega_3} d\omega_4 + \int d\omega_4 \int^{\omega_4} d\omega_3$$

Also in higher order iterations, *there is always a smallest integration variable* ω_i. Before and after it all the scattering events may occur, and the integral-eqns. *exactly* are turned into

$$T^0(z+\omega_1, z+\omega_2, z) + V^2 P_\sigma(z+\omega_1+\omega_2) = \int d\omega N(\omega) f(\omega)$$
$$\times \quad T^0(z+\omega_1, z+\omega, z) P_0(z+\omega) T^0(z+\omega, z+\omega_2, z)$$

2.) The integration variable ω is now the smallest one in all iterations of the integrals belonging to the two T^0's on the right hand side of the noninear integral eqn.. Thus it appears also *in the linear integral eqns. for the two* $T^0(\cdots)$ as lower limit. This procedure seems to work

in many more cases than the usual one, which turns the nonlinear integral eqn. into nonlinear differential equations of the Riccati-type, which are unsolvable for general inhomogeneities.

$$
\begin{aligned}
& T^0(z+\omega, z+\omega_2, z) + V^2 P_\sigma(z+\omega+\omega_2) \\
&= \quad -\int_\omega d\bar{\omega} T^0(z+\bar{\omega}, z+\omega_2, z) I^0(z+\omega, z+\bar{\omega}, z),
\end{aligned}
$$

In the *slow variable approximation* (SVA) one neglects ω besides $\bar{\omega}$ in

$$
\begin{aligned}
I^0(z+\omega, z+\bar{\omega}, z)) &= V^2 N(\bar{\omega}) f(\bar{\omega}) P_0(z+\bar{\omega}) P_\sigma(z+\bar{\omega}+\omega) \\
&\approx V^2 N(\bar{\omega}) f(\bar{\omega}) P_0(z+\bar{\omega}) P_\sigma(z+\bar{\omega})
\end{aligned}
$$

This is justified, if the propagator shows threshold behavior with a

threshold exponent between 0 and 1. Other possibility: Replace ω by $\bar{\omega}$, which is numerically equivalent. The last integral equation is then turned into a general 1st order differential equation, to be solved with the initial condition $T^0(z, z+\omega_2, z) = -V^2 P_\sigma(z+\omega_2)$. The solution reads

$$
\begin{aligned}
&T^0(z+\omega, z+\omega_2, z) + V^2 P_\sigma(z+\omega+\omega_2) = \\
&= \quad V^2 \int_0^\omega du P_\sigma(z+u+\omega_2) \frac{\partial}{\partial u} e^{\int_u^\omega dv I^0(z,z+v,z)}
\end{aligned}
$$

This and the corresponding solution for $T^0(z+\omega_1, z+\omega, z)$ is inserted into the nonlinear integral eqn.; and one proceeds similarly for the two other scattering matrices, thus obtaining a full *formal* solution for the scattering matrices in terms of the still unknown propagators.

Comparison with the numerical solution

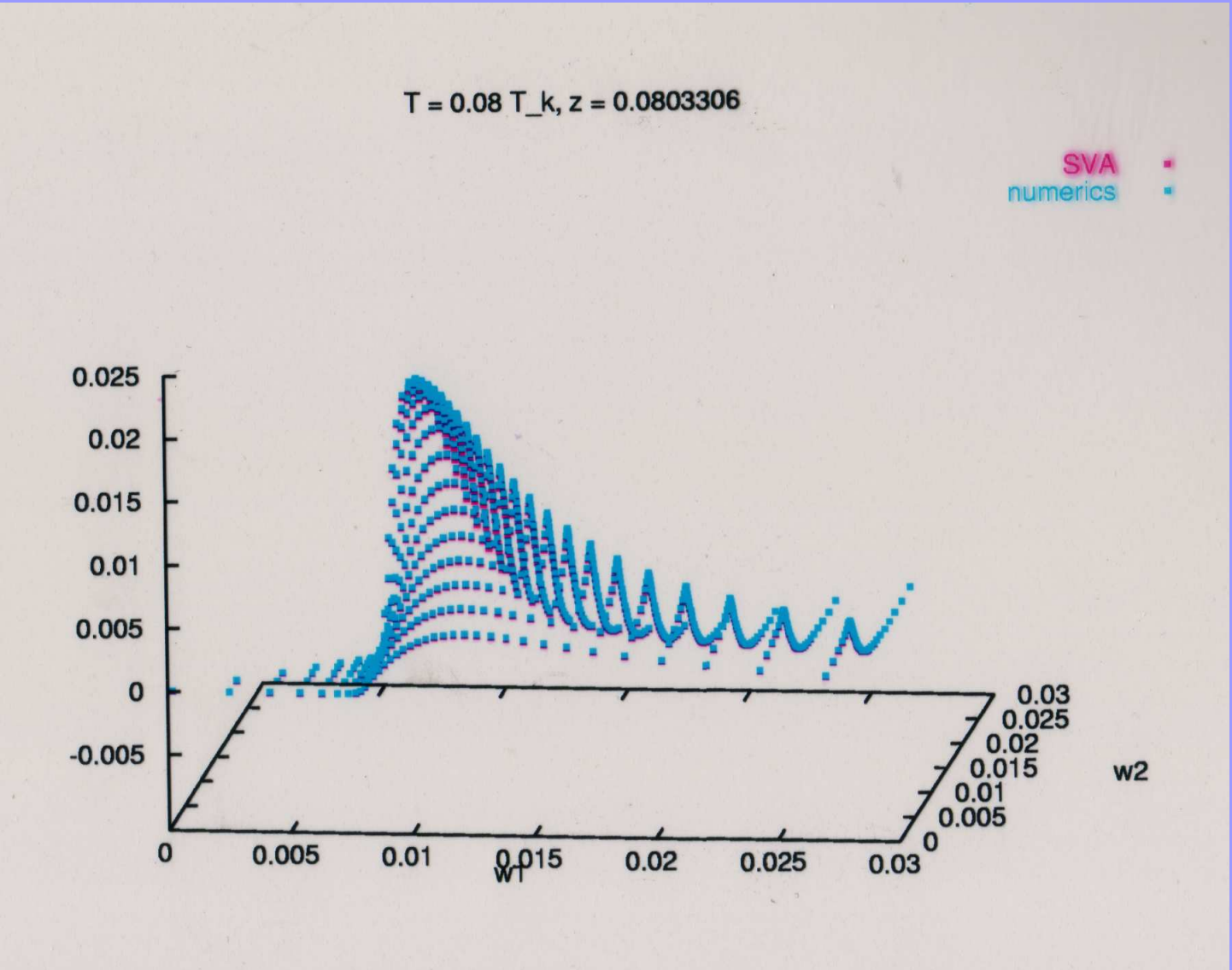
Matrix inversion with self adapting nets (and an improved inverse iteration, if necessary) are the heart of coming to grips with the CTMA integral eqs.. Slope and curvature compatibility is taken into account, following G.P. Lepage, J.Comput. Phys. **27** 192 (1978).
The goal is:
To obtain the 1st quantitative comparison between a slow variable approximation and the numerical results.
Steps in the numerical iteration:

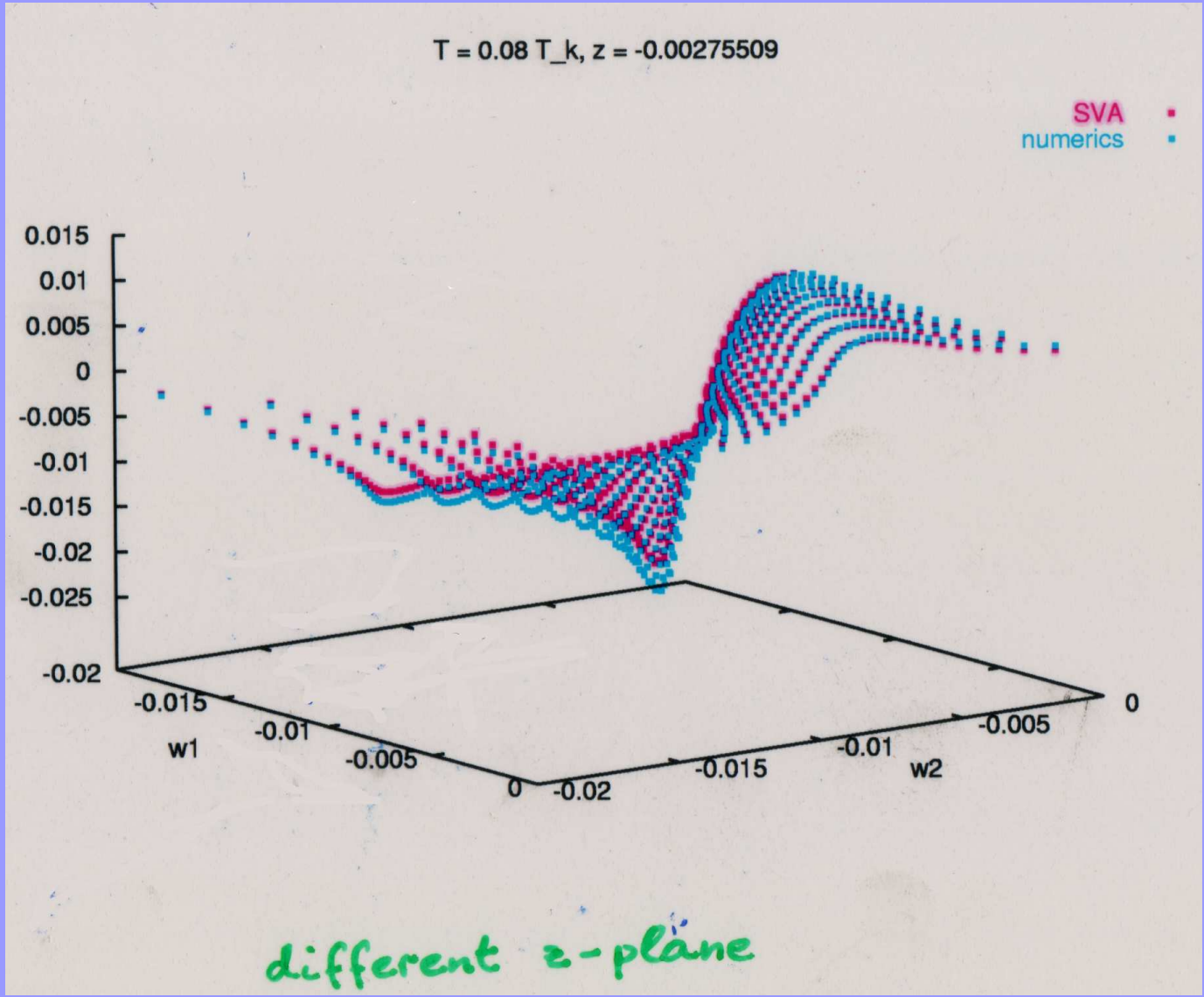
- Free propagators with a constant imaginary part, for which the sum rules are obeyed.
- Insert into scattering matrices and vertex functions
- Correct NCA
- Start with corrected propagators again.

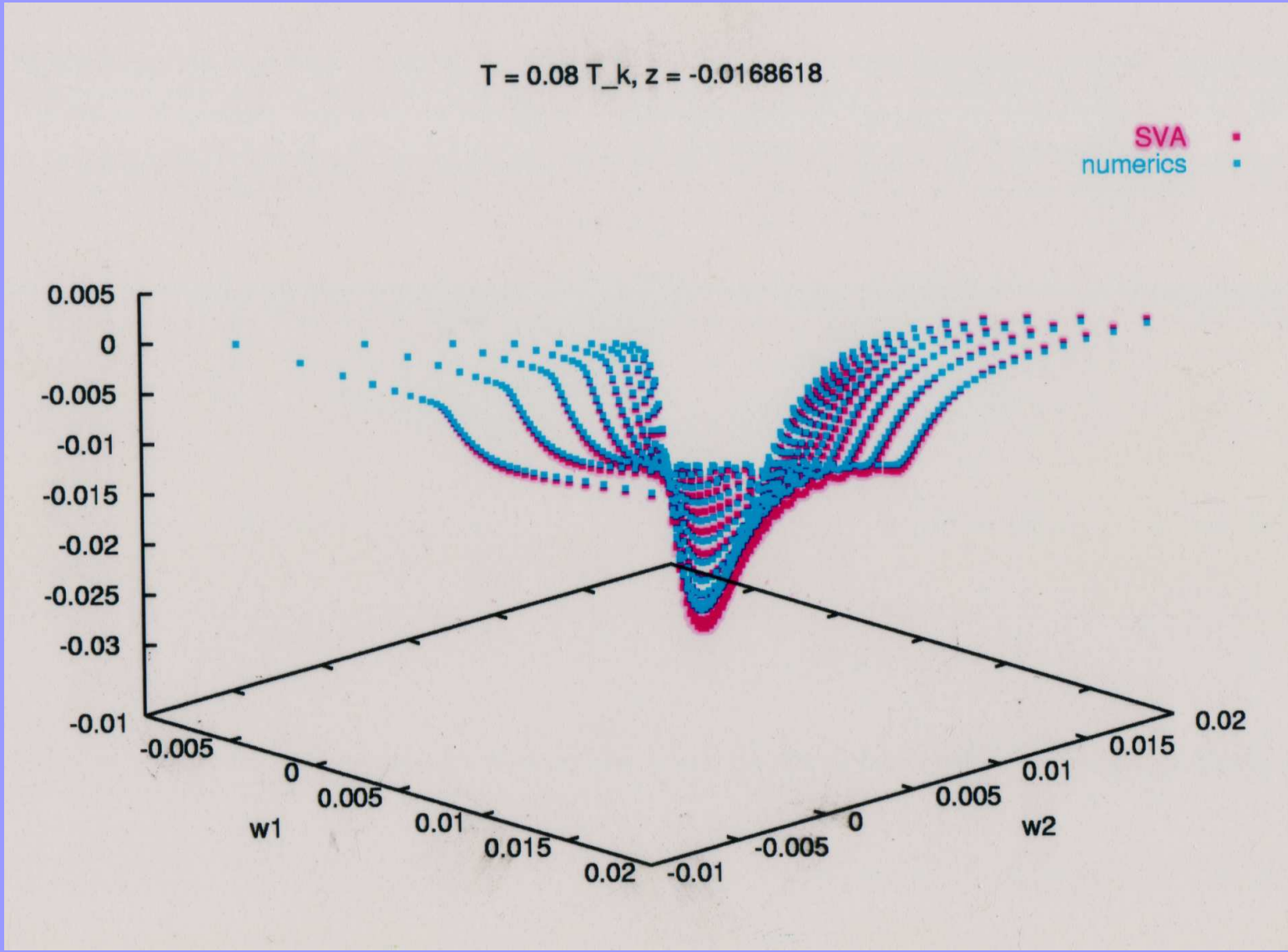
Use self adaptive nets (in C++). For ω_1 and ω_2 use 50 sample points between $-0.1eV$ and $0.1eV$, i.e bandwidth $= 0.2eV$, for the z-planes use 1000 between $-0.5eV \leq \Re z \leq 0.5eV$. Distribute them on the nodes of a parallel processor.
Aviod typical difficulties with factors like $e^{-\beta z}$ by multiplying with a suitable function.
Use effective vertices and scattering matrices.
In the following numerical results for the scattering matrices,

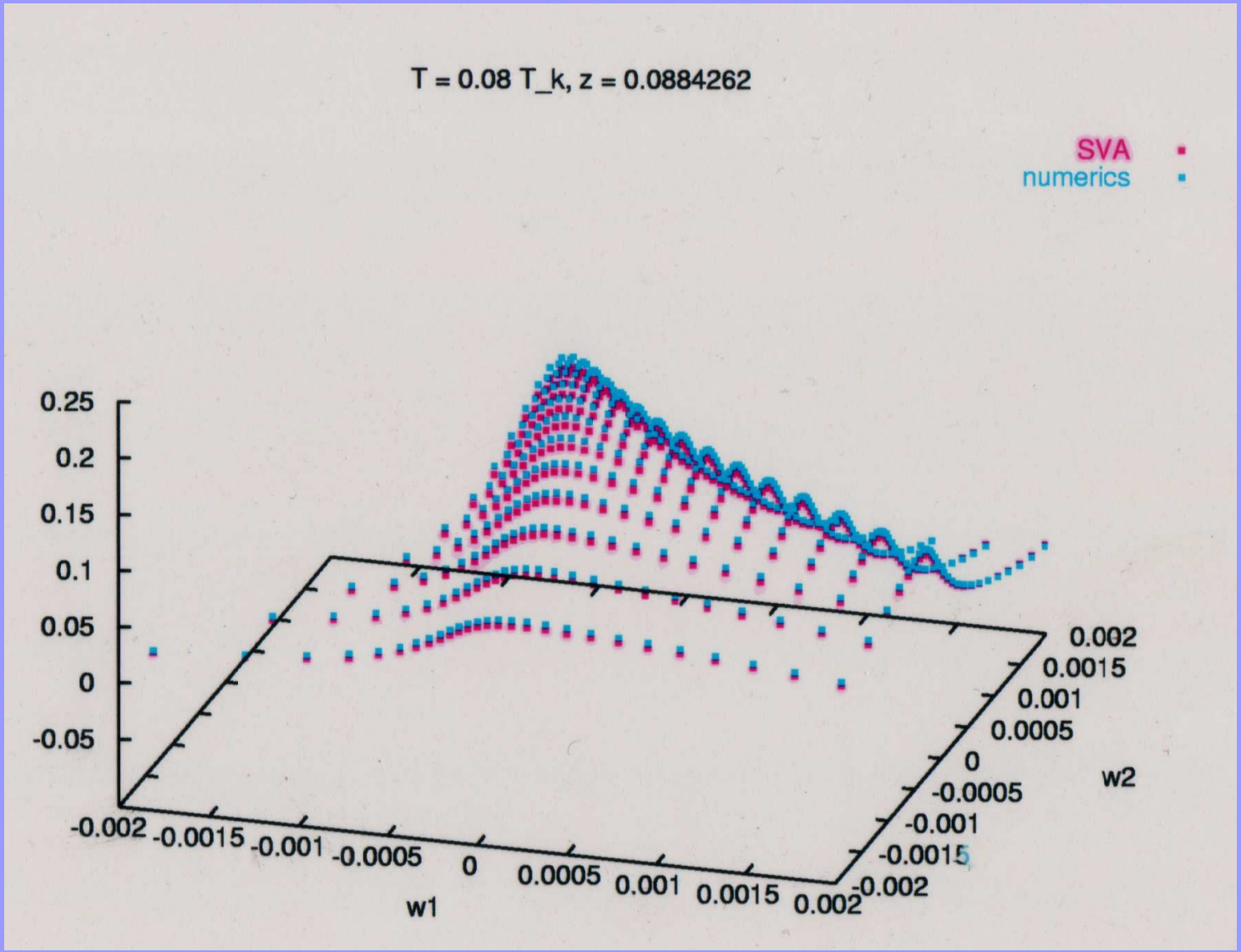
$$\Im[T^0(z+\omega_1, z+\omega_2, z) + V^2 P_\sigma(z+\omega_1+\omega_2)]$$

at fixed z as a function of ω_1, ω_2 are plotted in *eV*. $T_K = 20K \equiv 0.0017eV$. The agreement between the numerics and the SVA (in red) is really good.


T = 0.08 T_k, z = 0.0803306
SVA
numerics
0.025
0.02
0.015
0.01
0.005
0
-0.005
0
0.005
0.01
0.015
0.02
0.025
0.03
w1
0.03
0.025
0.02
0.015
0.01
0.005
0
w2

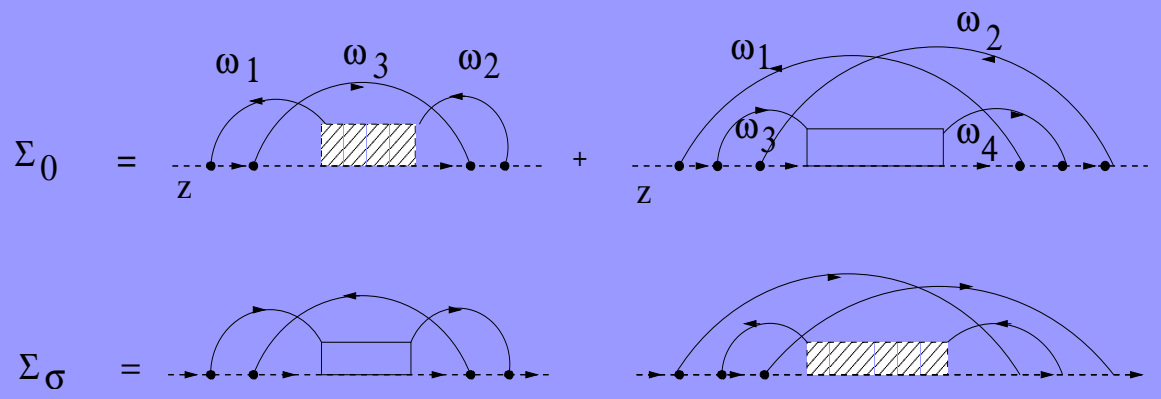

T = 0.08 T_k, z = -0.00275509
SVA
numerics
0.015
0.01
0.005
0
-0.005
-0.01
-0.015
-0.02
-0.025
-0.02
-0.015
-0.01
-0.005
0
w1
-0.02
-0.015
-0.01
-0.005
0
w2
different z-plane


T = 0.08 T_k, z = -0.0168618
SVA
numerics
0.005
0
-0.005
-0.01
-0.015
-0.02
-0.025
-0.03
-0.01
-0.005
0
0.005
0.01
0.015
0.02
w1
-0.01
-0.005
0
0.005
0.01
0.015
0.02
w2


T = 0.08 T_k, z = 0.0884262
SVA
numerics
0.25
0.2
0.15
0.1
0.05
0
-0.05
-0.002
-0.0015
-0.001
-0.0005
0
0.0005
0.001
0.0015
0.002
w1
0.002
0.0015
0.001
0.0005
0
-0.0005
-0.001
-0.0015
-0.002
w2

Self-consistence

From the scattering matrices one calculates $\Sigma_0(z)$ and $\Sigma_\sigma(z)$ as shown in the diagrams



The hatched box in $\Sigma_0(z)$ is $T^0(z+\omega_1-\omega_3, z+\omega_2-\omega_3, z-\omega_3)$.
The empty box in $\Sigma_0(z)$ is
$\frac{1}{2}[(T^+(z+\omega_1+\omega_2-\omega_3, z+\omega_1+\omega_2-\omega_4, z+\omega_1+\omega_2)+T^-(\cdots))\delta_{\sigma,\sigma'}$

$$+(T^+(\cdots)-T^-(\cdots))].$$

Then the self-energies are related to their propagators. In the numerics this is brought to convergence, after which $G_f(i\omega_n \to z)$ is calculated.

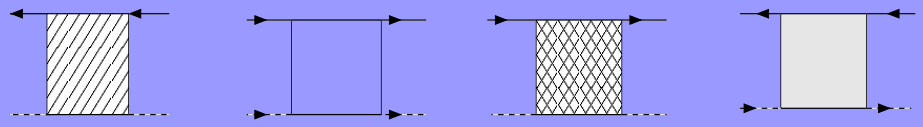
In the analytical approach a Ward identity is needed to treat the SVA to the scattering matrices on the same footing as the derivative of the Σ's. In view of the complicated connenctions between the T's and the Σ's this has not been achieved yet.

One of the two problems of the NCA is solved by the CTMA. Numerical evidence and perturbative renormalization group calculations show (S.Kirchner et al. Phys.Rev. **B70** 1655102 (2004) and J.Kroha, P.Wölfle J.Phys.Soc.Jap.**74** 16, (2005)) *that the threshold exponents show the expected dependence of the occupation of the f-level.*

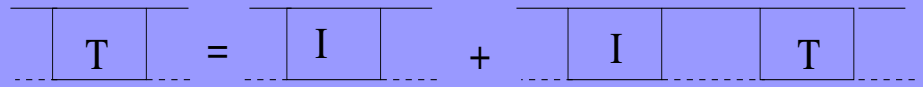
For the 2nd problem of the NCA, namely the correct treatment of the normal scattering potential in the Schrieffer-Wolff limit, and thus leading to Fermi-liquid behavior, *the CTMA fails*. This was 1st seen in the numerics (see e.g. the two papers above) and reconfirmed by one of us (K.B.), before the analytical treatmant showed that in 10th order the CTMA yields a normal scattering contribution which depends on temperature (S. Duffe, master thesis, in preparation.) In view of this, the empirical procedure used in the two papers above, seems reasonable: A normal potential is added, such that Fermi-liquid behavior is regained. The addition of a suitable normal potential shifts the peak in the spectral function of the f-electrons to the Fermi-level.

Parquet-type integral eqns.

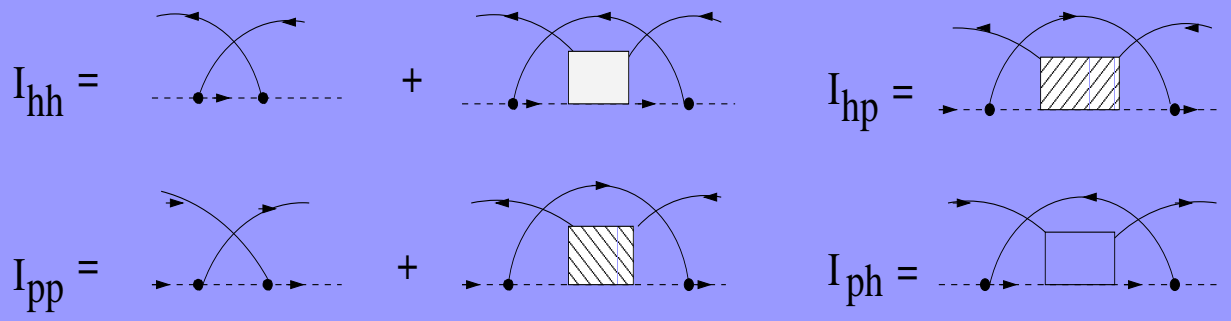
Why does the CTMA fail? Apparently one needs to treat direct and exchange processes on the same footing - i.e. to look for coupled Bethe-Salpeter eqns..
There are two further scattering channels, the last two in the following figure:



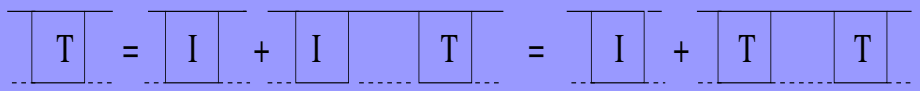
The scattering matrices are denoted by T_{hh},T_{pp},T_{ph}, and I_{hp}. The equations for them are of the Bethe-Salpeter type (arrows left off, initial, intermediate and final states must be the same):



Inspecting the scattering matrices, arising from cutting electron lines in the self-energy contributions with 4 vertices crossed in the generating functional, one guesses the following couplings



The full scattering matrix T_{hp} enters into the inhomogeneity I_{hh}. The I_{hp} contains the full scattering matrix T_{hh}. The same holds true, if h and p are interchanged. So the CTMA with *uncoupled* Bethe Salpeter equations is replaced by *coupled parquet-like equations.* Can one formally solve them?
Sudakov's trick works for any Bethe-Salpeter eqn., as seen from the following picture



The straight line between the last two boxes carries the lowest frequency. So the 1st step for the solution works.
For the 2nd step one again considers the linear integral equation. e.g. for $T_{hh} = T^0(z+\omega, z+\omega_2, z)$

$$-T^0(z+\omega, z+\omega_2, z) - I_{hh}(z+\omega, z+\omega_2, z) =$$
$$\int_\omega d\bar{\omega} T^0(z+\bar{\omega}, z+\omega_2, z) N(\bar{\omega}) f(\bar{\omega}) P_0(z+\bar{\omega}) I_{hh}(z+\omega, z+\bar{\omega}, z)$$

SVA:

$$I_{hh}(z+\omega, z+\bar{\omega}, z) = I_{hh}(z, z+\bar{\omega}, z)$$

Initial condition

$$T^0(z, z+\omega_2, z) = -I_{hh}(z, z+\omega_2, z)$$

Solution:

$$T^0(z+\omega, z+\omega_2, z) + I_{hh}(z+\omega, z+\omega_2, z) =$$
$$\int_0^\omega du I_{hh}(z+u, z+\omega_2, z) \times$$
$$\frac{\partial}{\partial u} e^{\int_u^\omega dv N(v) f(v) P_0(z+v) I_{hh}(z,z+v,z)}$$

Similar solutions for the other amplitudes T_{hp}, T_{pp}, T_{ph}.
Remainig problem (status at 28/09/05 16.00):

- T_{hh} and T_{hp} are still coupled, so are T_{pp} and T_{ph}. How to decouple them?

- Find a *Ward-identity* for the z-derivative of the self-energies and the scattering amplitudes.

- Numerical work on the new equations.

- For the *Ward-identity* exploit the connection between the self-energies andthe scattering matrices: