A Selfenergy Cookbook — State-of-the-Art Computing for the NEGF Key Ingredient

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KBEt^2, *Kiel*
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Equations of Motion for the NEGF

$$\sum_l \left[\mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}z_1} \delta_{il} - h_{il}\big(z_1\big) \right] G_{lj}\big(z_1, z_2\big) = \delta_{\mathcal{C}}\big(z_1, z_2\big)\delta_{ij} + \sum_l \int_{z_3} \Sigma_{il}\big(z_1, z_3\big) G_{lj}\big(z_3, z_2\big)$$

$$\sum_l G_{il}\big(z_1, z_2\big) \left[-\mathrm{i}\hbar \frac{\overleftarrow{\mathrm{d}}}{\mathrm{d}z_2} \delta_{lj} - h_{lj}\big(z_2\big) \right] = \delta_{\mathcal{C}}\big(z_1, z_2\big)\delta_{ij} + \sum_l \int_{z_3} G_{il}\big(z_1, z_3\big) \Sigma_{lj}\big(z_3, z_2\big)$$

$$\Sigma^{\mathrm{xc}}_{ij}\big(z_1, z_2\big) = \mathrm{i}\hbar \sum_{mpq} w_{ipqm}\big(z_1\big) \int_{\mathcal{C}} \mathrm{d}z_3 \sum_n G_{mn}\big(z_1, z_3\big) \Lambda_{nqpj}\big(z_3, z_2, z_1\big)$$

$$\Lambda_{ijkl}\big(z_1, z_2, z_3\big) = \delta_{\mathcal{C}}\big(z_1, z_{2+}\big)\delta_{\mathcal{C}}\big(z_3, z_2\big)\delta_{ik}\delta_{jl} + \int_{\mathcal{C}} \mathrm{d}z_4 \mathrm{d}z_5 \sum_{mn} \frac{\delta \Sigma_{il}\big(z_1, z_2\big)}{\delta G_{mn}\big(z_4, z_5\big)} \int_{\mathcal{C}} \mathrm{d}z_6 \sum_p G_{mp}\big(z_4, z_6\big) \int_{\mathcal{C}} \mathrm{d}z_7 \sum_q G_{qn}\big(z_7, z_5\big) \Lambda_{pjkq}\big(z_6, z_7, z_3\big)$$

$$G_{ij}\big(z_1, z_2\big) = G^{(0)}_{ij}\big(z_1, z_2\big) + \int_{\mathcal{C}} \mathrm{d}z_3 \mathrm{d}z_4 \sum_{mn} G^{(0)}_{im}\big(z_1, z_3\big) \Sigma_{mn}\big(z_3, z_4\big) G_{nj}\big(z_4, z_2\big)$$

$$W^{\mathrm{ns}}_{ijkl}\big(z_1, z_2\big) = \sum_{mn} w_{imnl}\big(z_1\big) \int_{\mathcal{C}} \mathrm{d}z_3 \sum_{pq} P_{nqpm}\big(z_1, z_3\big) W_{pjkq}\big(z_3, z_2\big)$$

$$\Sigma^{\mathrm{xc}}_{ij}\big(z_1, z_2\big) = \mathrm{i}\hbar \int_{\mathcal{C}} \mathrm{d}z_3 \sum_{mpq} W_{ipqm}\big(z_1, z_3\big) \times \int_{\mathcal{C}} \mathrm{d}z_4 \sum_n G_{mn}\big(z_1, z_4\big) \Gamma_{nqpj}\big(z_4, z_2, z_3\big)$$

$$P_{ijkl}\big(z_1, z_2\big) = \pm \mathrm{i}\hbar \int_{\mathcal{C}} \mathrm{d}z_3 \sum_m G_{im}\big(z_1, z_3\big) \times \int_{\mathcal{C}} \mathrm{d}z_4 \sum_n G_{nl}\big(z_4, z_1\big) \Gamma_{mjkn}\big(z_3, z_4, z_2\big)$$

$$\Gamma_{ijkl}\big(z_1, z_2, z_3\big) = \delta_{\mathcal{C}}\big(z_1, z_{2+}\big)\delta_{\mathcal{C}}\big(z_3, z_2\big)\delta_{ik}\delta_{jl} + \int_{\mathcal{C}} \mathrm{d}z_4 \mathrm{d}z_5 \sum_{mn} \frac{\delta \Sigma^{\mathrm{xc}}_{il}\big(z_1, z_2\big)}{\delta G_{mn}\big(z_4, z_5\big)} \int_{\mathcal{C}} \mathrm{d}z_6 \sum_p G_{mp}\big(z_4, z_6\big) \int_{\mathcal{C}} \mathrm{d}z_7 \sum_q G_{qn}\big(z_7, z_5\big) \Gamma_{pjkq}\big(z_6, z_7, z_3\big)$$

$$\sum_l \left[\mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}z_1}\delta_{il} - h_{il}(z_1) \right] G_{lj}(z_1, z_2) = \delta_{\mathcal{C}}(z_1, z_2)\delta_{ij} + \sum_l \int_{z_3} \Sigma_{il}(z_1, z_3) G_{lj}(z_3, z_2)$$

$$\sum_l G_{il}(z_1, z_2) \left[-\mathrm{i}\hbar \frac{\overleftarrow{\mathrm{d}}}{\mathrm{d}z_2}\delta_{lj} - h_{lj}(z_2) \right] = \delta_{\mathcal{C}}(z_1, z_2)\delta_{ij} + \sum_l \int_{z_3} G_{il}(z_1, z_3)\Sigma_{lj}(z_3, z_2)$$

$$G_{ij}(z_1, z_2) = G^{(0)}_{ij}(z_1, z_2) + \int_{\mathcal{C}} \mathrm{d}z_3 \mathrm{d}z_4 \sum_{mn} G^{(0)}_{im}(z_1, z_3)\Sigma_{mn}(z_3, z_4) G_{nj}(z_4, z_2)$$

$$W^{\mathrm{ns}}_{ijkl}(z_1, z_2) = \sum_{mn} w_{imnl}(z_1) \int_{\mathcal{C}} \mathrm{d}z_3 \sum_{pq} P_{nqpm}(z_1, z_3) W_{pjkq}(z_3, z_2)$$

$$\Sigma^{\mathrm{xc}}_{ij}(z_1, z_2) = \mathrm{i}\hbar \int_{\mathcal{C}} \mathrm{d}z_3 \sum_{mpq} W_{ipqm}(z_1, z_3) \times \int_{\mathcal{C}} \mathrm{d}z_4 \sum_n G_{mn}(z_1, z_4)\Gamma_{nqpj}(z_4, z_2, z_3)$$

$$\Sigma^{\mathrm{xc}}_{ij}(z_1, z_2) = \mathrm{i}\hbar \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} \mathrm{d}z_3 \sum_n G_{\dots}(z_{\dots}, z_{\dots})\Lambda_{\dots}(z_{\dots}, z_{\dots}, z_{\dots})$$

$$P_{\dots}(z_1, z_2) = \pm \mathrm{i}\hbar \int_{\mathcal{C}} \mathrm{d}z_3 \sum_m G_{im}(z_1, z_3) \times \int_{\mathcal{C}} \mathrm{d}z_4 \sum_n G_{nl}(z_4, z_1)\Gamma_{mjkn}(z_3, z_4, z_2)$$

$$\Lambda_{ijkl}(z_1, z_2, z_3) = \delta_{\mathcal{C}}(z_1, z_2)\delta_{\mathcal{C}}(z_3, z_2)\dots + \int_{\mathcal{C}} \mathrm{d}z_4 \mathrm{d}z_5 \sum_{mn} \frac{\delta\Sigma_{il}(z_1, z_2)}{\delta G_{mn}(z_4, z_5)} \int_{\mathcal{C}} \mathrm{d}z_6 \sum_p G_{mp}(z_4, z_6) \int_{\mathcal{C}} \mathrm{d}z_7 \sum_q G_{qn}(z_7, z_5)\Lambda_{pjkq}(z_6, z_7, z_3)$$

$$\Gamma_{ijkl}(z_1, z_2, z_3) = \delta_{\mathcal{C}}(z_1, z_2)\delta_{\mathcal{C}}(z_3, z_2)\delta_{ik}\delta_{jl} + \int_{\mathcal{C}} \mathrm{d}z_4 \mathrm{d}z_5 \sum_{mn} \frac{\delta\Sigma^{\mathrm{xc}}_{il}(z_1, z_2)}{\delta G_{mn}(z_4, z_5)} \int_{\mathcal{C}} \mathrm{d}z_6 \sum_p G_{mp}(z_4, z_6) \int_{\mathcal{C}} \mathrm{d}z_7 \sum_q G_{qn}(z_7, z_5)\Gamma_{pjkq}(z_6, z_7, z_3)$$

Central Quantity: Selfenergy Σ

Going beyond Second Born – Selfenergy Overview

Computational Remarks

The Hubbard model

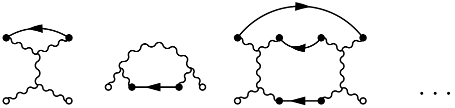
Performance Tests

Feynman Diagrams

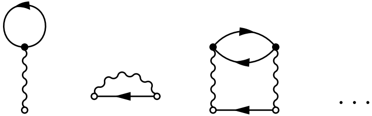
- Use Feynman diagrams to visualize Green functions and interactions
- general vs. diagonal basis:

$G_{ij}(z, z') =$ 

$w_{ijkl}(z, z') =$ 

$\rightarrow$ 

$w_{ij}(z, z') =$ 

$\rightarrow$ 

- Hartree–Fock selfenergy becomes:

$$\Sigma_{ij}^{\mathrm{HF}}(z, z') = \pm \mathrm{i}\hbar \delta_{\mathcal{C}}(z, z') \sum_{k,l} \int_{\mathcal{C}} \mathrm{d}\bar{z}\, w_{iklj}(z, \bar{z}) G_{lk}(\bar{z}, \bar{z}^+) + \mathrm{i}\hbar \sum_{k,l} w_{ikjl}(z, z') G_{lk}(z, z'^+)$$

$\rightarrow$  $\mapsto \pm \mathrm{i}\hbar$  $+ \mathrm{i}\hbar$ 

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selfenergy approximations that solve the Martin–Schwinger hierarchy can be derived from a closed set of equations

two equivalent, formally exact approaches based on:

– the **screened** interaction/vertex:

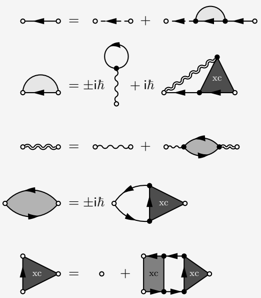
$$G(1,2) = G^{(0)}(1,2) + G^{(0)}(1,3)\Sigma(3,4)G(4,2)$$

$$\Sigma(1,2) = \pm i\hbar\delta(1,2)w(1,3)G(3,3^+) + i\hbar W(1,3)G(1,4)\Gamma(4,2,3)$$

$$W(1,2) = w(1,2) + w(1,3)P(3,4)W(4,2)$$

$$P(1,2) = \pm i\hbar G(1,3)G(4,1)\Gamma(3,4,2)$$

$$\Gamma(1,2,3) = \delta(1,2^+)\delta(3,2) + \frac{\delta\Sigma^{\text{xc}}(1,2)}{\delta G(4,5)}G(4,6)G(7,5)\Gamma(6,7,3)$$

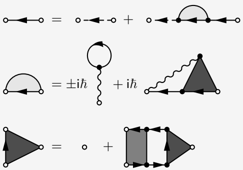


– the **bare** interaction/vertex:

$$G(1,2) = G^{(0)}(1,2) + G^{(0)}(1,3)\Sigma(3,4)G(4,2)$$

$$\Sigma(1,2) = \pm i\hbar\delta(1,2)w(1,3)G(3,3^+) + i\hbar w(1,3)G(1,4)\Lambda(4,2,3)$$

$$\Lambda(1,2,3) = \delta(1,2^+)\delta(3,2) + \frac{\delta\Sigma(1,2)}{\delta G(4,5)}G(4,6)G(7,5)\Lambda(6,7,3)$$



L. Hedin, Phys. Rev. **139**, A796 (1965).

quick & easy

SOA, 2B

Second-Order (Born) Approximation

- all diagrams up to second order in the interaction
- easiest way to include correlation effects
- combination with the GKBA $\rightarrow N_t^2$-scaling
- applicable to a wide range of systems

Computation

simple matrix multiplication

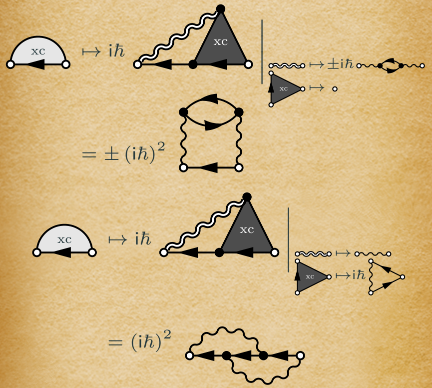
Numerical Scaling

- general basis: $\mathcal{O}\left(N_t^2 N_b^5\right)$
- diagonal basis: $\mathcal{O}\left(N_t^2 N_b^4\right)$

Accuracy Range

- **weak** to **moderate** coupling
- no filling dependence

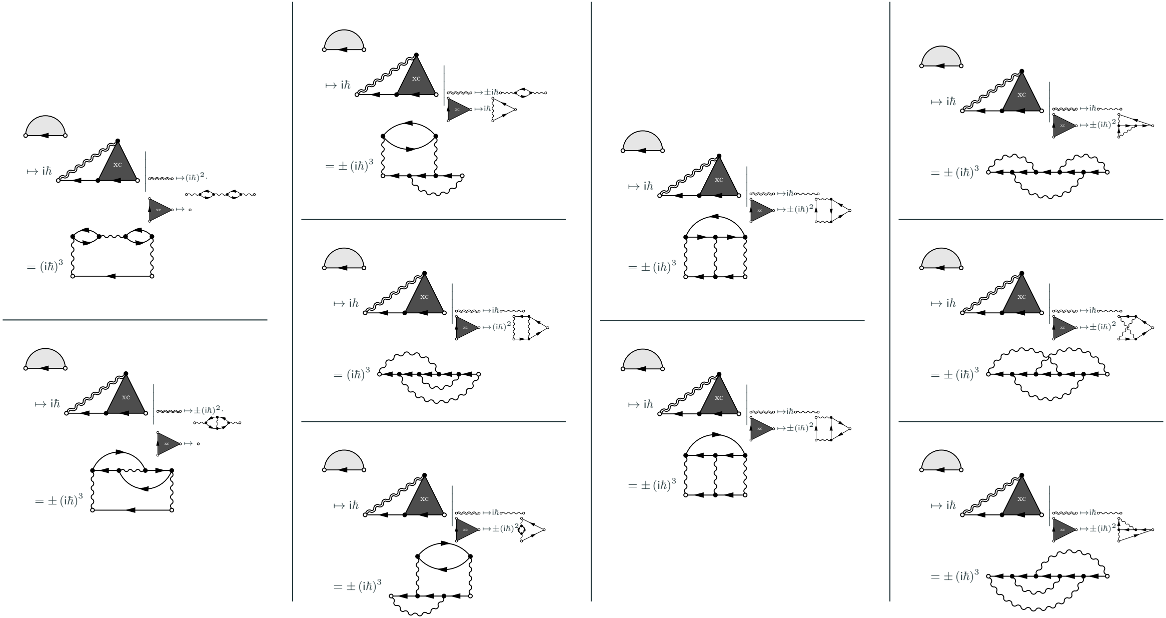
from **screened** approach:



$$\Sigma^{(2)}\left(1,2\right)$$
$$= \pm\left(\mathrm{i}\hbar\right)^2 w\left(1,3\right) G\left(3,4\right) G\left(4,3\right) w\left(4,2\right) G\left(1,2\right)$$
$$+ \left(\mathrm{i}\hbar\right)^2 w\left(1,3\right) G\left(1,4\right) w\left(4,2\right) G\left(4,3\right) G\left(3,2\right)$$

Third-Order Diagrams

Derivation of third-order terms from Hedin's equations (screened approach):



N. Schlünzen, S. Hermanns, M. Scharnke, and M. Bonitz, submitted, arXiv:1902.07038 (2019).

the nitpicker

TOA

Third-Order Approximation

- all diagrams up to third order in the interaction
- more involved calculation
- applicability range restricted to moderate basis size

Computation

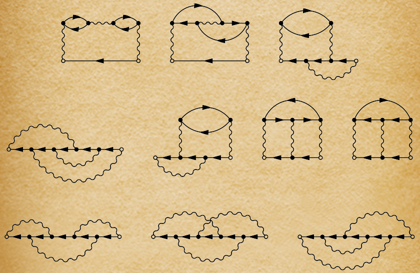
matrix multiplication +
numerical integration

Numerical Scaling

- general basis: $\mathcal{O}\left(N_t^3 N_b^5\right)$
- diagonal basis: $\mathcal{O}\left(N_t^3 N_b^4\right)$

Accuracy Range

- **moderate** to **strong** coupling
- no filling dependence



$$
\begin{aligned}
&\Sigma^{(3)}\left(1,2\right)\\
&= \left(\mathrm{i}\hbar\right)^3 G\left(1,2\right) w\left(1,3\right) G\left(3,4\right) G\left(4,3\right) w\left(4,5\right) G\left(5,6\right) G\left(6,5\right) w\left(6,2\right)\\
&\quad \pm \left(\mathrm{i}\hbar\right)^3 w\left(1,3\right) G\left(3,5\right) G\left(6,3\right) w\left(5,6\right) G\left(5,4\right) G\left(4,6\right) w\left(4,2\right) G\left(1,2\right)\\
&\quad \pm \left(\mathrm{i}\hbar\right)^3 w\left(1,5\right) G\left(5,6\right) G\left(6,5\right) w\left(6,3\right) G\left(1,4\right) w\left(4,2\right) G\left(4,3\right) G\left(3,2\right)\\
&\quad + \left(\mathrm{i}\hbar\right)^3 w\left(1,3\right) G\left(1,4\right) w\left(4,2\right) G\left(4,5\right) G\left(6,2\right) w\left(5,6\right) G\left(5,3\right) G\left(3,6\right)\\
&\quad \pm \left(\mathrm{i}\hbar\right)^3 w\left(1,3\right) G\left(1,4\right) w\left(4,6\right) G\left(6,7\right) G\left(7,6\right) w\left(7,2\right) G\left(4,3\right) G\left(3,2\right)\\
&\quad + \left(\mathrm{i}\hbar\right)^3 w\left(1,3\right) G\left(1,4\right) w\left(4,6\right) w\left(5,2\right) G\left(5,6\right) G\left(6,2\right) G\left(4,3\right) G\left(3,5\right)\\
&\quad \pm \left(\mathrm{i}\hbar\right)^3 w\left(1,3\right) G\left(1,4\right) w\left(4,6\right) G\left(6,5\right) w\left(5,2\right) G\left(4,2\right) G\left(5,3\right) G\left(3,6\right)\\
&\quad + \left(\mathrm{i}\hbar\right)^3 w\left(1,3\right) G\left(1,4\right) w\left(4,6\right) w\left(5,2\right) G\left(5,6\right) G\left(6,2\right) G\left(4,3\right) G\left(3,5\right)\\
&\quad + \left(\mathrm{i}\hbar\right)^3 w\left(1,3\right) G\left(1,4\right) w\left(4,6\right) G\left(4,5\right) w\left(5,2\right) G\left(6,2\right) G\left(5,3\right) G\left(3,6\right)\\
&\quad + \left(\mathrm{i}\hbar\right)^3 w\left(1,3\right) G\left(1,4\right) w\left(4,5\right) G\left(4,6\right) w\left(6,2\right) G\left(6,5\right) G\left(5,3\right) G\left(3,2\right)
\end{aligned}
$$

it all comes down to bubbles

GWA

GW Approximation

- easiest way to decribe dynamical-screening effects
- sums up polarization-bubble diagram series
- computationally demanding, but scaling advantage for diagonal basis sets

Computation

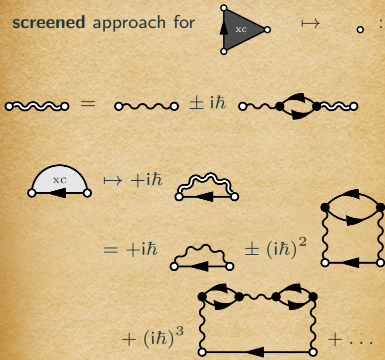
matrix multiplication + numerical integration, solution by **iteration** or **inversion**

Numerical Scaling

- general basis: $\mathcal{O}\left(N_t^3 N_b^6\right)$
- diagonal basis: $\mathcal{O}\left(N_t^3 N_b^3\right)$

Accuracy Range

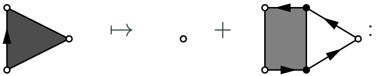
- **moderate** to **strong** coupling
- around **half filling**



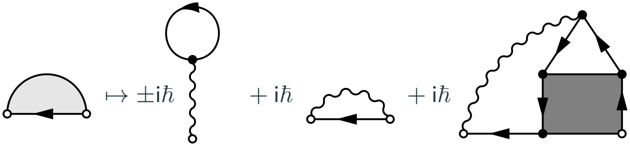
$$W\left(1,2\right)$$
$$= w\left(1,2\right) \pm \mathrm{i}\hbar w\left(1,3\right)G\left(3,4\right)G\left(4,3\right)W\left(4,2\right)$$
$$\Sigma^{GW}\left(1,2\right) = \Sigma^{\mathrm{H}}\left(1,2\right) + \mathrm{i}\hbar G\left(1,2\right)W\left(1,2\right)$$

Getting the T Matrices from the Bare Approach

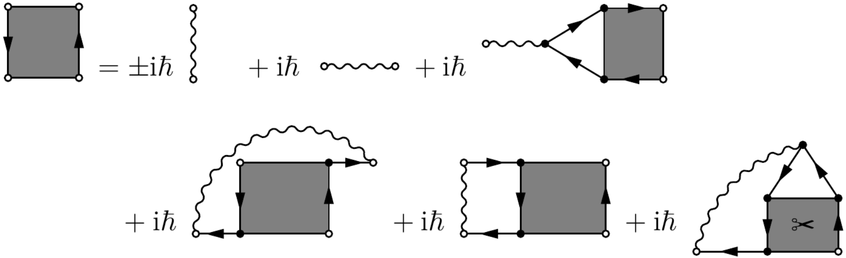
Truncation of the **bare**-vertex recursion by



The selfenergy becomes:



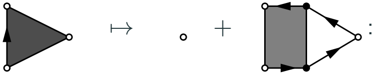
The selfenergy derivative starts off three diagram series:



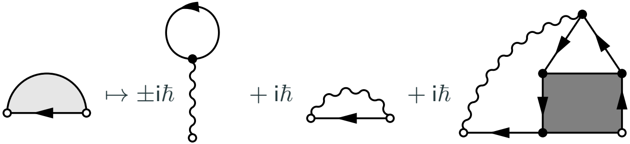
N. Schlünzen, S. Hermanns, M. Scharnke, and M. Bonitz, submitted, arXiv:1902.07038 (2019).

Getting the T Matrices from the Bare Approach

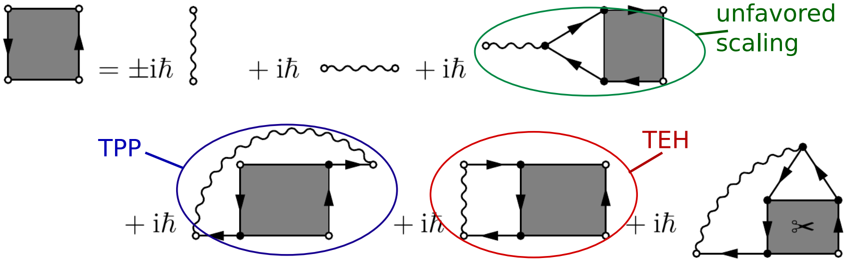
Truncation of the **bare**-vertex recursion by



The selfenergy becomes:



The selfenergy derivative starts off three diagram series:



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climbing the ladder I

TPP

Particle–Particle
***T*-Matrix** Approximation

- sums up the diagrams of the Born series
- computationally expensive → applicable only to moderate basis size
- becomes exact in the limit of low (large) density

Computation

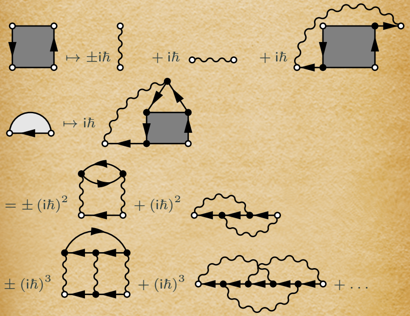
matrix multiplication + numerical integration, solution by **iteration** or **inversion**

Numerical Scaling

- general basis: $\mathcal{O}\left(N_t^3 N_b^6\right)$
- diagonal basis: $\mathcal{O}\left(N_t^3 N_b^6\right)$

Accuracy Range

- **moderate** to **strong** coupling
- **low**/**large** density



$$T^{\mathrm{pp}}\left(1,2\right) = w\left(1\right)G\left(1,2\right)G\left(1,2\right)w^{\pm}\left(2\right) + w\left(1\right)G\left(1,3\right)G\left(1,3\right)T^{\mathrm{pp}}\left(3,2\right)$$

$$\Sigma^{\mathrm{TPP}}\left(1,2\right) = \mathrm{i}\hbar T^{\mathrm{pp}}\left(1,2\right)G\left(2,1\right)$$

climbing the ladder II

TPH, TEH

Particle (Electron)–Hole
***T*-Matrix** Approximation

- sums up a series of particle–hole diagrams
- computationally demand and reach similar to TPP
- specifically designed to describe systems around half half filling

Computation

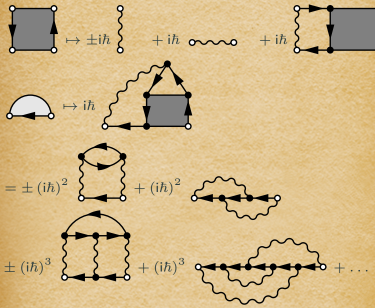
matrix multiplication + numerical integration, solution by **iteration** or **inversion**

Numerical Scaling

- general basis: $\mathcal{O}\left(N_t^3 N_b^6\right)$
- diagonal basis: $\mathcal{O}\left(N_t^3 N_b^6\right)$

Accuracy Range

- **moderate** to **strong** coupling
- around **half filling**



$$T^{\mathrm{ph}}\left(1,2\right) = w\left(1\right)G\left(1,2\right)G\left(2,1\right)w^{\pm}\left(2\right) + w\left(1\right)G\left(1,3\right)G\left(3,1\right)T^{\mathrm{ph}}\left(3,2\right)$$

$$\Sigma^{\mathrm{TPH}}\left(1,2\right) = i\hbar T^{\mathrm{ph}}\left(1,2\right)G\left(2,1\right)$$

it's a matter of patience

FLEX

Fluctuating-Exchange Approximation

- merges the diagram series of the TPP, the TPH and the GWA
- combines advantages of its ingredients
- highest computational demands of the presented approximations

Computation

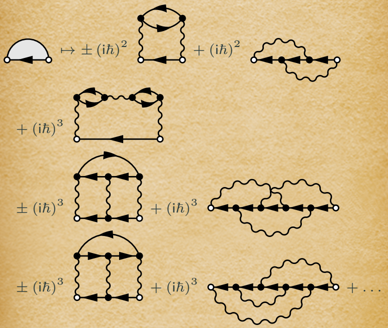
matrix multiplication + numerical integration, solution by **iteration** or **inversion**, avoid double counting of mutual terms

Numerical Scaling

- general basis: $\mathcal{O}\left(N_t^3 N_b^6\right)$
- diagonal basis: $\mathcal{O}\left(N_t^3 N_b^6\right)$

Accuracy Range

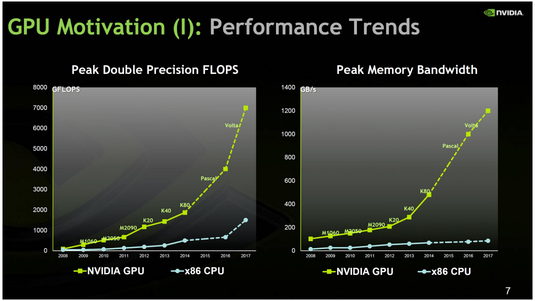
- **moderate** to **strong** coupling
- no filling dependence

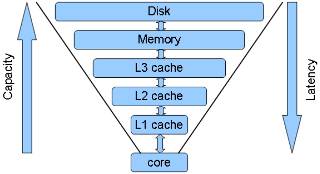


$$\Sigma^{\mathsf{FLEX}}\left(1,2\right) = \Sigma^{(1)}\left(1,2\right) + \Sigma^{GW,\mathsf{corr}}\left(1,2\right) + \Sigma^{\mathsf{TPP,corr}}\left(1,2\right) + \Sigma^{\mathsf{TPH,corr}}\left(1,2\right) - 2\Sigma^{(2)}\left(1,2\right)$$

Computational Remarks

- **high-performance** computing and massive **parallelization** are essential to outgrow toy models
- NEGF is **well-suited**, contains high degree of independent calculations in matrix multiplication and numerical integration
- possible with multi-core programming on multiple CPUs
- “cheaper” way ⇒ parallelization on GPUs
- con: memory structure is hard to manage

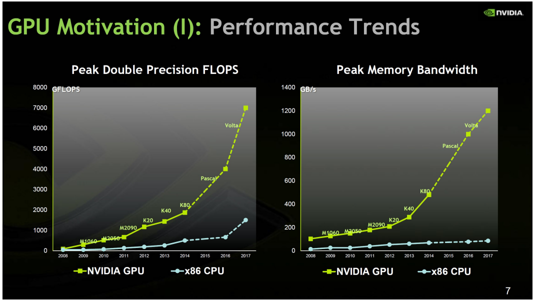


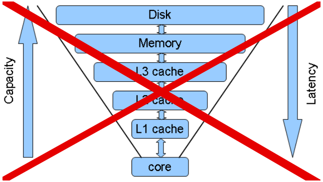


HTTPS://WCCFTECH.COM/NVIDIA-PASCAL-GPU-ANALYSIS/

Computational Remarks

- **high-performance** computing and massive **parallelization** are essential to outgrow toy models
- NEGF is **well-suited**, contains high degree of independent calculations in matrix multiplication and numerical integration
- possible with multi-core programming on multiple CPUs
- "cheaper" way ⇒ parallelization on GPUs
- con: memory structure is hard to manage
- salvation: unified memory since NVIDIA Pascal!





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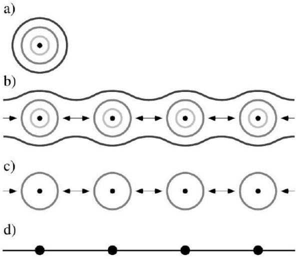
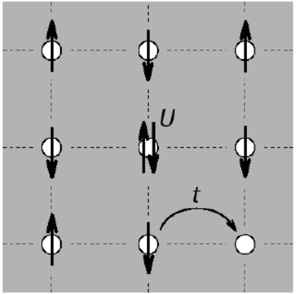
- Going beyond Second Born – Selfenergy Overview
- Computational Remarks
- The Hubbard model
- Performance Tests



$\Longrightarrow$

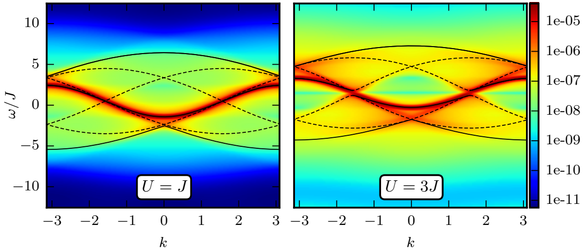


$$\hat{H}(t) = J\sum_{ij,\,\alpha} h_{ij}\,\hat{c}^\dagger_{i\alpha}\hat{c}_{j\alpha} + U\sum_i \hat{c}^\dagger_{i\uparrow}\hat{c}_{i\uparrow}\hat{c}^\dagger_{i\downarrow}\hat{c}_{i\downarrow} + \sum_{ij,\alpha\beta} f_{ij,\alpha\beta}(t)\,\hat{c}^\dagger_{i\alpha}\hat{c}_{j\beta}$$

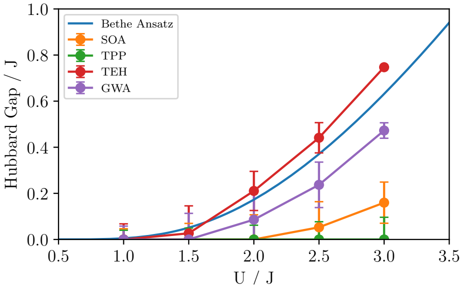
$h_{ij} = -\delta_{\langle i,\,j\rangle}$ and $\delta_{\langle i,\,j\rangle} = 1$, if (i,j) nearest neighbors, $\delta_{\langle i,\,j\rangle} = 0$ otherwise;
on-site repulsion ($U > 0$) or attraction ($U < 0$), U favors *doublons* (correlations)

- f: excitation (1-particle hamiltonian): EM field, quench, particle impact etc.
- finite inhomogeneous system, size and geometry dependence

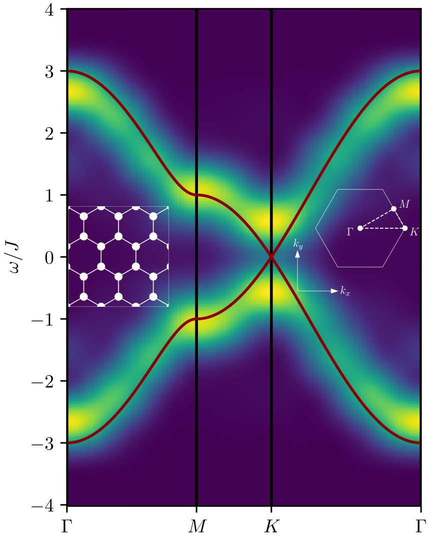
dispersion of 40-site Hubbard chain (2B/SOA):



band gap for the infinite 1D chain:



band structure for the honeycomb lattice:



J.-P. Joost, N. Schlünzen, and M. Bonitz, phys. stat. sol. (b), doi: 10.1002/pssb.201800498, (2019)

Computational Scaling

- N_t: number of time steps, N_b: basis size

- scaling of propagation scheme
  - full KBE: $\mathcal{O}\left(N_t^3\right)$, $\mathcal{O}\left(N_b^3\right)$
  - HF-GKBA: $\mathcal{O}\left(N_t^2\right)$, $\mathcal{O}\left(N_b^3\right)$

- scaling of selfenergy approximations:

	HF	2B	TOA	GW	TPP	TEH	FLEX	
order	$\sim w^1$	$\sim w^2$	$\sim w^3$	$\to w^\infty$				
N_t-scaling	$\mathcal{O}\left(N_t^1\right)$	$\mathcal{O}\left(N_t^2\right)$	$\mathcal{O}\left(N_t^3\right)$					
N_b-scaling	$\mathcal{O}\left(N_b^4\right)$	$\mathcal{O}\left(N_b^5\right)$		$\mathcal{O}\left(N_b^6\right)$				$\boldsymbol{w_{ijkl}}$
	$\mathcal{O}\left(N_b^2\right)$	$\mathcal{O}\left(N_b^4\right)$		$\mathcal{O}\left(N_b^3\right)$	$\mathcal{O}\left(N_b^6\right)$			$\boldsymbol{V_{ij} := w_{ijij}}$
	$\mathcal{O}\left(N_b^1\right)$	$\mathcal{O}\left(N_b^2\right)$	$\mathcal{O}\left(N_b^3\right)$					$\boldsymbol{U_i := w_{iiii}}$

- lattice models greatly reduce numerical complexity

Selfenergy Approximations in the Hubbard Model

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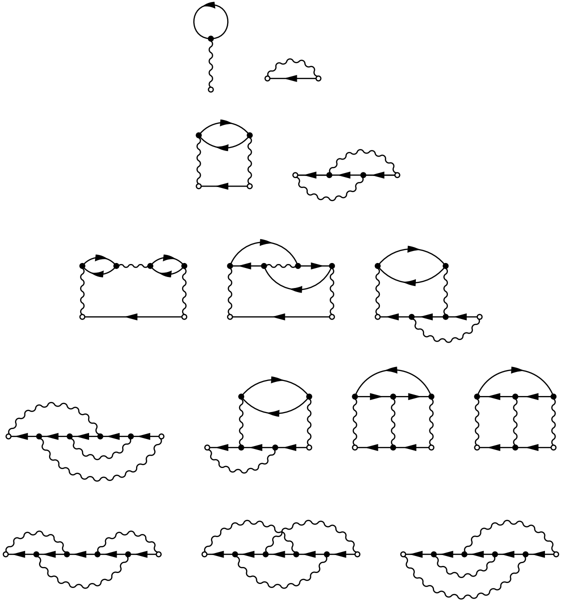
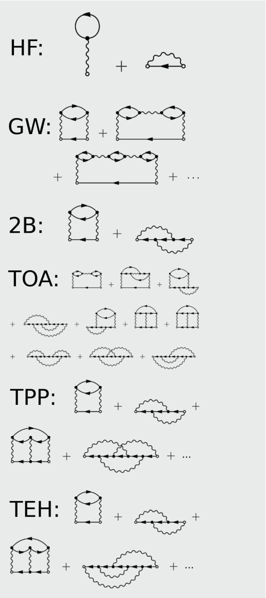
Mathematisch-Naturwissenschaftliche Fakultät





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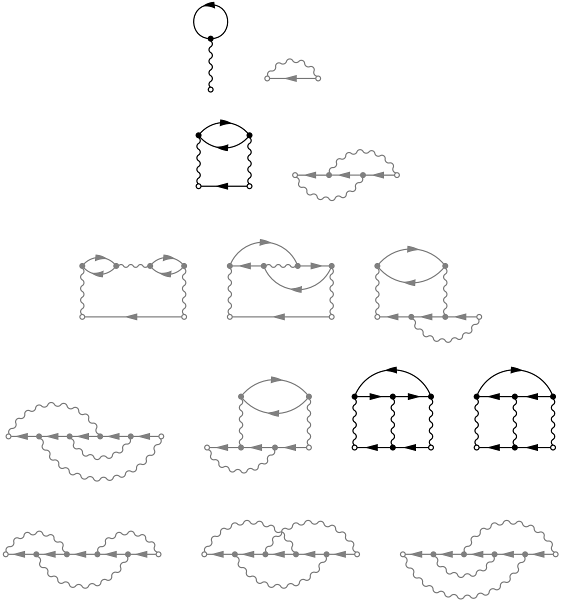

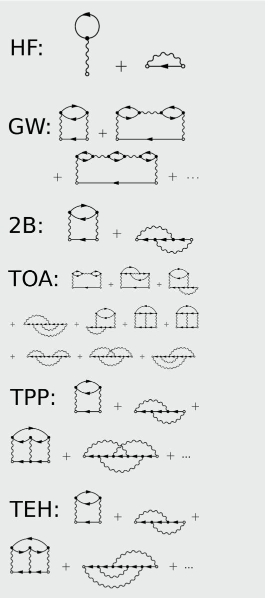

Selfenergy Approximations in the Hubbard Model

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Christian-Albrechts-Universität zu Kiel
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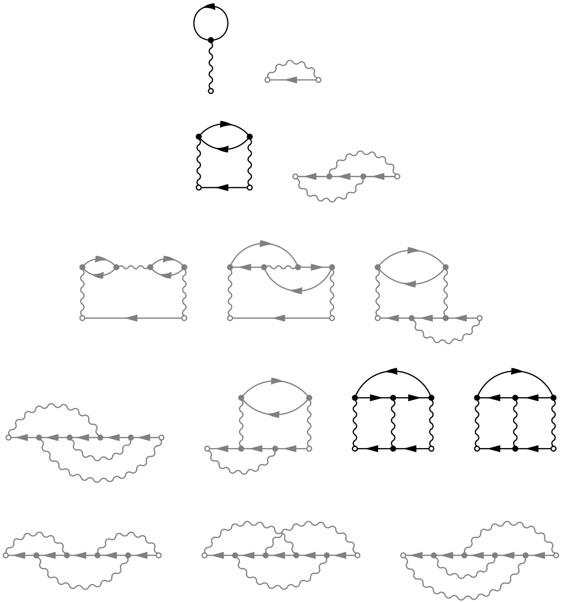
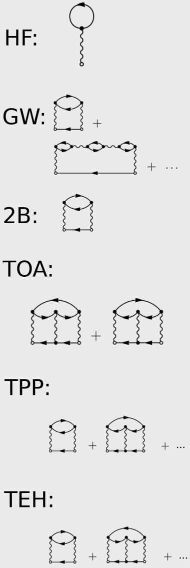
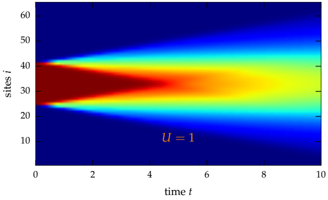




Performance Test: Interaction – Expansion



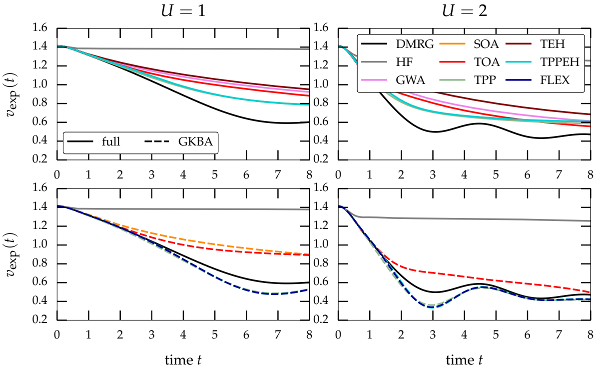
- Hartree–Fock misses the slowing-down of the expansion
- trend: two-time propagation results underestimate the slowing-down
- best performance by TPP, TPPEH, FLEX combined with GKBA

- initial state: doubly occupied sites at the center
- Hubbard chain of 65 sites with 34 particles
- non-trivial expansion, U-dependent
- mean squared displacement

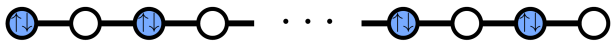
$$R^2(t) = \frac{1}{N}\sum_{\boldsymbol{s}} n_{\boldsymbol{s}}(t)[\boldsymbol{s}-\boldsymbol{s}_0]^2$$

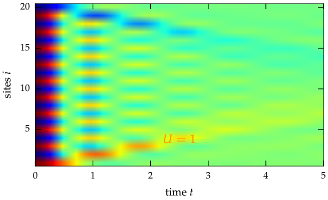
$\boldsymbol{s}_0$: center of the system

- rescaled cloud **diameter** $d(t) = \sqrt{R^2(t) - R^2(0)}$
- **expansion velocity** $v_{\mathrm{exp}}(t) = \frac{\mathrm{d}}{\mathrm{d}t} d(t)$



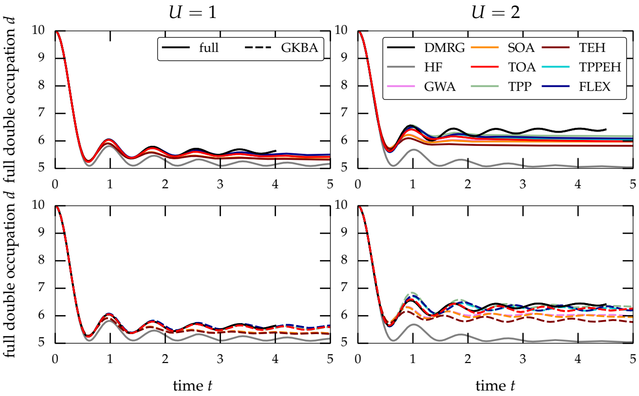
Performance Test: Interaction – Relaxation CDW



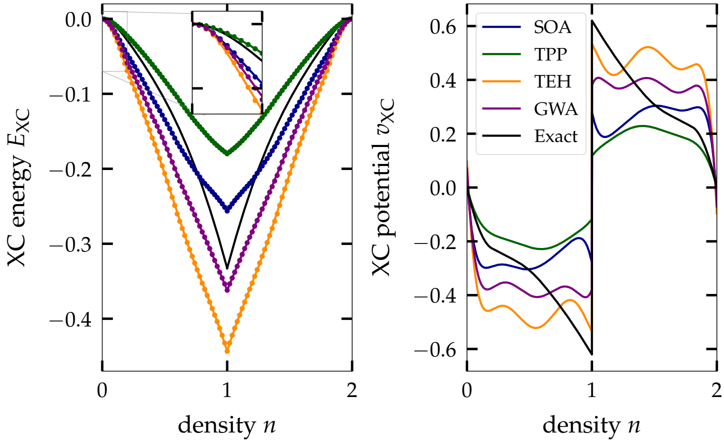


- Hartree–Fock results are not sufficient
- two-time results become steady due to artificial damping
- best performance by GKBA+TOA

- initial state: doubly occupied sites arranged as a charge density wave
- Hubbard chain of 20 sites with 20 particles
- Relaxation dynamics towards homogeneous density distribution
- fast build-up of correlations
- observables: double occupation



Results for a ten-site Hubbard chain for the $U = 4J$ ground state:



low/high density:

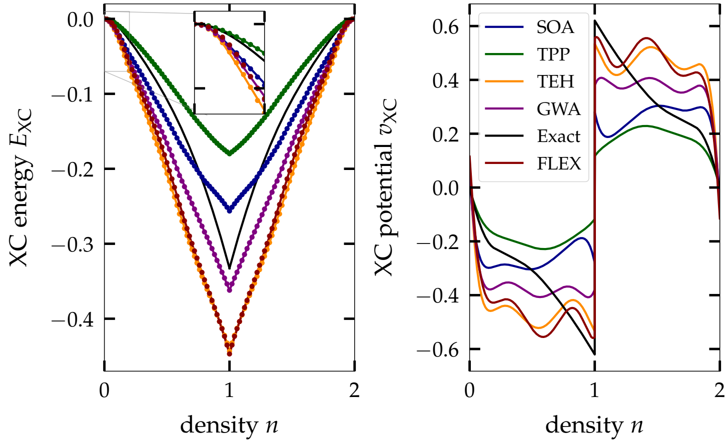
- **SOA**, **GWA** and **TEH** slightly off
- **excellent** agreement for the **TPP**

around half filling:

- **TPP** and **SOA** fail and underestimate band gap
- **GWA** becomes strikingly **accurate**
- **TEH** slightly overestimates correlations, precise band gap

Performance Test: Density

Results for a ten-site Hubbard chain for the $U = 4J$ ground state:



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- **SOA**, **GWA** and **TEH** slightly off
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- **TPP** and **SOA** fail and underestimate band gap
- **GWA** becomes strikingly **accurate**
- **TEH** slightly overestimates correlations, precise band gap

FLEX dominated by TEH, no significant improvement

no “allrounders” ⇒ physical circumstances prescribe the best choice of Σ

- in many cases **Second Born** is **not sufficient** to describe correlations accurately
- going beyond SOA is not straight forward $\Rightarrow$ **no "allrounders"**
- controlled choice of selfenergy: **dictated** by **filling** and **interaction** strength, accurate up to $U \simeq$ bandwidth
- best performance by
  - low/large filling: TPP
  - half filling: GWA, TEH
  - mixed nonequilibrium: TOA
- Hubbard basis drastically reduces numerical effort by scaling and diagram number
- **parallelization** is crucial and can be done on GPUs

Appendix

Finite Band Gap – Size Dependence