Dynamical competition between disorder and interactions in ultracold atoms and transport phenomena

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DFT meets QIT, Araraquara, 17th December 2014
Plan of the Talk

- Disorder
  - Still a major theme in condensed matter physics
  - Relevant to QIT as a source of noise and source of decay of correlations (e.g. Burrell and Osborne, 2007)
  - Revival in cold atoms: engineering disorder
  - Difficult problem: even adiabatic-type approaches can offer insight

- Approach I: NEGF
  - 2nd Born for interactions (but also GW and TMA to test approximations)
  - Numerical treatment of disorder and Coherent Potential Approximation (CPA)

- Approach II: lattice (TD)DFT
  - XC potential via DMFT

APPLIED TO

- 3D optical lattices with fermions.
  - Benchmarking DMFT-ALDA: KBE vs. TDDFT vs. exact dynamics in small 3D clusters
  - Expansion of fermion clouds in ordered and disordered lattices in TDDFT-DMFT

- 1D quantum transport geometries.
  - Transport via NEGF in disordered Hubbard chains at Finite Bias
Disorder and interactions

**No interactions**

1D  All eigenstates localized for any nonzero disorder. Conductance decays exponentially with system size.

2D  Localization for any nonzero disorder. For weak disorder, localization length is very large.

3D  Above critical disorder value, all states localized. *No complete rigorous theory for Anderson localization.*

**LDOS indicator of the MIT**

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**Minimal model WITH INTERACTIONS**

\[
H = \sum_{ij\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i\sigma} \epsilon_i n_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}
\]

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**Our motivation here**

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**Interactions ?**

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**Experiment:** evidence of MIT in 2D Resistivity $\rho$ in a dilute low-disorder Si MOSFET as function of electron density $n$ and temperature $T$. At low $T$, $\rho$ increases (decreases) at lower (higher) $n$, a sign of insulating (conducting) behavior.
One approach: NEGF
Kadanoff-Baym Equations

- **Basic quantity**
  \[ G(12) = -i \langle T_C \left[ \hat{\psi}_H(1) \hat{\psi}^+_H(2) \right] \rangle \]

- **Dyson Equation in time**
  \[ (i \partial_{t_1} - h(t_1)) G(t_1, t_2) = \delta(t_1, t_2) + \int_C \Sigma(t_1, t) G(t, t_2) \, dt \]

- **Conserving approximations:**
  \[ \Sigma = \Sigma[G] \quad \text{functional derivative of generating functionals} \]

- **Time propagation:** time square

- **In the presence of leads**
  \[\Sigma = \Sigma_{MB}^{C C} + \Sigma_{emb} \]
  \[\Sigma_{emb} = \sum_{\alpha=L,R} |V_{C\alpha}|^2 g_{\alpha\alpha}\]

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Kadanoff and Baym (1962); Keldysh, JETP (1965); Danielewicz (1984); Jauho et al (1994); Kohler et al (1999); Kwong and Bonitz (2000); Stefanucci and Almbladh (2004); Myhöhänen et al., (2008)
K. Balzer and M. Bonitz’s book, Springer (2013),
Many Body Approximations:

\[ \Sigma_{TMA}(12) = \Sigma_{HF} + iU^2 G(21) T(12) \]
\[ T = \phi - \phi U T, \quad \phi(12) = -i G(12) G(12) \]

Example

Tested against static and dynamical exact solutions for Hubbard/Anderson clusters

Recently: GKBA Hermanns et al 2013-14

Finite systems & conserving MBA:s artificially damped dynamics (Puig, CV, Almbladh, 2009)
The other approach: TDDFT
- LDA for the XC potential via DMFT
### LATTICE DFT

<table>
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<tr>
<th>Year</th>
<th>Authors</th>
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<tr>
<td>1986-88</td>
<td>Gunnarsson and Schönhammer</td>
<td>General idea</td>
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<td>1995</td>
<td>Schönhammer, Gunnarsson, Noack</td>
<td>LDA for the 1D Hubbard model via Bethe-Ansatz</td>
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<td>2002-03</td>
<td>Lima, Silva, Oliveira, Capelle</td>
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<td>2008</td>
<td>Franca and Capelle</td>
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<td>2011</td>
<td>Karlsson, Privitera, Verdozzi</td>
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<td>2012</td>
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### Lattice TDDFT

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<tr>
<td>2008</td>
<td>Verdozzi</td>
<td>General idea; Exact $v_{xc}$ in Hubbard chains; ALDA for lattice TDDFT</td>
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<td>2008</td>
<td>Baer, Li and Ullrich, Verdozzi</td>
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<td>2013-14</td>
<td>Fuks et al</td>
<td>Non-adiabatic effects and charge transfer in Hubbard dimers</td>
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<td>2014</td>
<td>Mancini et al,</td>
<td>The role of local approximations</td>
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<tr>
<td>2012</td>
<td>Farzanehpour and Tokatly</td>
<td>TDDFT for QED on a lattice</td>
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### Time-dependent quantum transport

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<td>2010</td>
<td>Kurth et al.</td>
<td>Coulomb Blockade in TD transport</td>
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<td>2011</td>
<td>Uimonen et al.</td>
<td>TDDFT vs tDMRG vs NEG</td>
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<tr>
<td>2011</td>
<td>Bergfield et al., Stefanucci and Kurth, Troster, Evers, Schmitteckert</td>
<td>(TD)DFT and the Kondo regime in transport</td>
</tr>
</tbody>
</table>
Other work

For DFT see also:
2008: Franca and Capelle
entanglement
2010: Akande and Sanvito
electric polarization
2010: Ijäs and Harju
graphene lattice
2011: Carrascal and Ferrer
small systems
2012: Lorenzana et al.
DFT with pair-densities
2012: Perfetto and Stefanucci
attractive interactions
2013: Lorenzana and Brosco
XC potential at the surface

For TDDFT see Also:
2002: Aryasetiawan et al.
linear response in a lattice
2004: Magyar et al.
linear response in a lattice
2010 : Puig et al.
v_{xc} from MBA:s
2011: Karlsson et al.
1D cold-fermion atoms
2012: Turkovsky and Rahman
Frequency-dependent XC kernel

Quantum Transport
2009: Dzierzawa et al.
current DFT for 1D Fermions
2011: Akande and Sanvito
Current DFT for disordered Hubbard rings
2011: Mirjani and Thijsse
spin dependent transport
2012: Pertsova et al
transport across a quantum dot
Lattice DFT and TDDFT for the Hubbard model

\[ H = -i \sum_{(ij)\sigma} a_{i\sigma}^{\dagger} a_{j\sigma} + \sum_i U \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} + \sum_{i\sigma} v_{ext}(i, \tau) \hat{n}_{i\sigma} \]

The total energy

\[ E[n, v_{ext}] = E_0[n] + E_H[n] + E_{xc}[n] + \sum_i v_{ext}(i)n_i \]

\[ \frac{E(n,U)}{L} = -\frac{2\beta(U)}{\pi} \sin \left( \frac{\pi n}{\beta(U)} \right) \]

\[ -\frac{2\beta(U)}{\pi} \sin \left( \frac{\pi}{\beta(U)} \right) = -4 \int_0^\infty dx \frac{J_0(x)J_1(x)}{x[1 + \exp(Ux/2)]} \]

The XC potential

\[ v_{xc} = \frac{\partial e_{xc}(n,U)}{\partial n} \]

The KS equations

\[ (\hat{\imath} + \hat{v}_{KS}) \varphi_\kappa = \varepsilon_\kappa \varphi_\kappa \]

\[ v_{KS} = v_H + v_{xc} + v_{ext} \]

The LDA

\[ v_{xc}(i) \approx v_{xc}^{\text{hom}}(n_i) \]

\[ n_i = \sum_\sigma n_{i\sigma} = 2 \sum_\kappa |\varphi_\kappa(i)|^2 \]
DFT /TDDFT for the 3D Hubbard model
(Karlsson, Privitera, CV, 2011)

\[ H = -t \sum_{\langle ij \rangle \sigma} a_i^+ a_j + \sum_i U \hat{n}_{i \uparrow} \hat{n}_{i \downarrow} + \sum_{i \sigma} v_{ext}(i, \tau) \hat{n}_{i \sigma} \]

\[ \nu_{xc}^{\text{hom}}(n) = \frac{\partial}{\partial n} (E_{DMFT}[n] - T_0[n] - U n^2/4), \]

Magnetic phases neglected: pure Mott physics

- Basic DMFT: HM in infinite dimensions.
- & exact mapping into single U impurity

\[ \nu_{xc} \text{ from DMFT} \]

\begin{tabular}{cccc}
\hline
\text{U=8} & \text{U=12} & \text{U=24} & \text{U=36} \\
\hline
\end{tabular}

\begin{center}
\begin{tikzpicture}
% Add your TikZ code here to draw the diagram
\end{tikzpicture}
\end{center}

- A discontinuity in \( \nu_{xc} \)
- Mott plateaus in cold atom clouds
- Coulomb Blockade in TD Quantum Transport
- A “spike” at \( n=1 \) in the XC kernel
- Kondo effect in KS conductance
- Mott-Hubbard Metal-Insulator Transition
Mott-Hubbard Metal-Insulator Transition within lattice DFT

The onset of a discontinuity in the XC potential reflects the MIT

\[ A(\omega) \]

\[ \nu_{xc}(n) \]

\[ U=4 \]

\[ U=8 \]

\[ U=24 \]

\[ U=36 \]

\[ \Delta > 0 \]

\[ \Delta = 0 \]

Cfr. the 1D case  gap at any nonzero interaction strength

(Karlsson, Privitera, CV, 2011)
Some benchmarks for TDDFT-DMFT-ALDA
Benchmarking ALDA-DMFT: TD density of one interacting impurity in the center of a 125-site cluster

**Interaction & perturbation only in the center**

**Exact propagation**
- Lanczos/Krylov technique

**KBE propagation**
- as discussed before

**TDDFT time propagation**
- KS eqs.  \((\hat{t} + \hat{v}_{KS}(\tau)) \varphi_\kappa(\tau) = i\partial_\tau \varphi_\kappa(\tau)\),
- with  \(v_{KS}(i, \tau) = v_H(i, \tau) + v_{xc}(i, \tau) + v_{ext}(i, \tau)\)
- ALDA  \(v_{xc}(i, \tau) \rightarrow v_{xc}^{DMFT}(n_{i}(\tau))\)
- with  \(n_i(\tau) = \sum_\kappa |\varphi_\kappa(i, \tau)|^2\)

by symmetry, a 10-site effective cluster
Benchmarking ALDA-DMFT

**TD density of the central site of a 5x5x5 cluster**

*Slow Gaussian pulse*

$$W_g = -5e^{-\frac{(\tau-5)^2}{2}}$$

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**U=8**

- Exact
- ALDA-DMFT
- BA
- GWA
- TMA

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**U=24**

*Weak, slow field*

KBE and ALDA-DMFT perform well

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*Strong, slow field:*

ALDA-DMFT performs well; KBE results inferior to ALDA-DMFT

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(CV, Karlsson, Puig, Almbladh, von Barth, Chem. Phys. 2011)
Benchmarking ALDA-DMFT  

**TD density of the central site of a 5x5x5 cluster**

**U=8, step potential**  \( W(\tau) = W_0 \Theta(\tau) \)

- **Fast and weak perturbation**
  - TMA and exact in very good agreement, ALDA: increasing dephasing

- **Fast and stronger perturbation**
  - TMA considerably better than ALDA
  - ALDA unreliable

- **Stronger interaction:**
  - KBE+MBPT and ALDA fail

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**Graphical Representation:**

- **Density at central site**
- **Time**
- **W_0=-0.2, W_0=-2**
Disorder and correlations in 3D: Expansion of Fermionic clouds
On the experimental side:

Fermionic transport and out-of-equilibrium dynamics in a homogeneous Hubbard model with ultracold atoms

Previous (TD)DFT work:
1D equilibrium: Xianlong et al, 2006
1D out-of-equilibrium: Karlsson, CV, Odahisma, Capelle, 2011
1D and spin resolved quenches: Gao Xianlong, 2011
Cold-Atoms: 3D Hubbard model in a parabolic trap

A cut across the $z=0$ plane of a cubic cluster $n(x, y | z = 0)$

(TD)DFT treatment for
- Clusters with up to $47^3$ sites
- Cloud expansion with disorder:
  i) $\sim 2000$ particles to propagate in time
  ii) Lanczos/Krylov time propagation

U=8, fast trap opening, no disorder

U = 8 sudden

U = 24 slow

U=24 slow

U=8, fast trap opening with disorder

T=0

T=3

T=6

quasi-typical random structure
Disorder enhances delocalization by additional escape pathways

Disorder and correlations in 1D: quantum transport geometries
**GENERAL OBSERVATIONS ABOUT DISORDER AND INTERACTIONS:**

Weak disorder weakens correlations

*Redistributes states into the Mott gap: insulator into a (bad) metal.*

Short-range interactions: transfer of spectral weight into the Hubbard subbands

*Total band-width increases, and thus critical disorder strength for the Anderson MIT*

Minimal model

\[
H = \sum_{ij} t_{ij} c_i^{\dagger} c_j + \sum_{i\sigma} \epsilon_i n_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}
\]

LDOS indicator of the MIT

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**How do interactions affect the picture? The Hubbard-Anderson model**

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**Do Interactions Increase or Reduce the Conductance of Disordered Electrons? It Depends!**

Thomas Vojta, Frank Epperlein, and Michael Schreiber

*Institut für Physik, Technische Universität, D-09107 Chemnitz, Germany*

(Received 16 June 1998)

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**Signatures of Delocalization in the Fermionic 1D Hubbard Model with Box Disorder: Comparative Study with DMRG and R-DMFT**

Julia Wernsdorfer, Georg Harder, Ulrich Schollwöck, and Walter Hofstetter

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**DC conductance for 5x5 sites**
Quantum transport in 1D disordered Hubbard chains (Karlsson and CV, PRB Rapid. Comm. 2014)

Chains with up to 10-15 sites; Diagonal box and binary disorder; Disorder averaging: numerical and CPA

\[ H = -t \sum_{\langle ij \rangle \sigma} a_{i\sigma}^\dagger a_{j\sigma} + \sum_{l \in C} [w_l \hat{n}_l + U \hat{n}_l \hat{n}_l] + \hat{W}_L(\tau) + \hat{W}_R(\tau) \]

\[ I_\alpha = \int_{-\infty}^{\infty} d\omega \frac{1}{2\pi i} \text{Tr} \{ \Gamma_\alpha(\omega) (G^{<}(\omega) - 2\pi i f_\alpha(\omega) A(\omega)) \} . \]

Steady state NEGF results with $\Sigma_{2B}$

The effect of interactions and disorder for bias $b_l = 0.5$. Results are for an $L=10$ chain a): Heat map for the current. b): Cuts along a fixed disorder strength (horizontal cuts in the heat map), as a function of $U$. c): Cuts along fixed interaction strength (vertical cuts) as a function of $W$. The legend applies to both a, b) panels.

- Near the $U=0$ ($W=0$) line, the current decreases monotonically as function of disorder (interactions).
- For intermediate interactions and/or disorder, the current is non-monotonic at finite bias.
- For any fixed value of $U$ the current monotonically decreases as a function of disorder strength.
Preliminary TMA results

The “disordered” dimer case in the TMA:

30 disorder configurations, bias=0.5 slow switch-on, half filling

Competition out of equilibrium
also within the KBE-TMA
Disorder averaging: non-equilibrium Coherent Potential Approximation

(Karlsson and Verdozzi, 2014)

In equilibrium, rigorous understanding from numerical studies. When out of equilibrium
i) expensive sums over configurations,
ii) extend to non-equilibrium analytical static treatments (e.g. CPA)
Out of equilibrium, “conservingness” not automatically guaranteed.

Equilibrium:
The CPA treats the disorder-averaged system by an effective medium, where $\langle T \rangle = 0$. Approximately, $\langle t_i(\omega) \rangle = 0$
The equilibrium CPA condition is ($V_i = \text{impurity level}$, $G_{ii}(\omega) = \text{averaged local propagator}$)

$$\langle t_i(\omega) \rangle = \left\langle \frac{V_i - \Sigma_{\text{CPA}}^{CPA}(\omega)}{1 - (V_i - \Sigma_{\text{CPA}}^{CPA}(\omega))G_{ii}(\omega)} \right\rangle = 0.$$ 

Non-Equilibrium:
CPA + DFT feasible.
NEGF with CPA + $\Sigma_{\text{MB}}$ lacking.
Proven conservation of current in CPA.

8-site chains with binary disorder. The applied bias $b_L=0.5$. CPA currents quantitatively incorrect, and qualitatively correct only for large disorder $W=3$. 
An entanglement perspective: single-site entanglement entropy
(Shannon-von Neumann entropy of four probabilities)

\[ \mathcal{E}_k = -2 \left( \frac{n_k}{2} - d_k \right) \log_2 \left( \frac{n_k}{2} - d_k \right) - d_k \log_2 d_k - (1 - n_k - d_k) \log_2 (1 - n_k - d_k) \]

\[ d_k = \frac{\partial e(n_k, U)}{\partial U} \]

\[ d_k = \frac{n_k^2}{4} + \frac{1}{U_k} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} \left( \Sigma_{MB}^{<} G^{A} + \Sigma_{MB}^{R} G^{<} \right)_{kk} \cdot \]

Example from finite system with ED, TMA and DFT-LDA

(DFT: Franca and Capelle, 2008)

(NEGF: Puig, CV, Almbladh, 2011)
Entanglement, disorder, and conductance  (Karlsson, CV, 2014)

Recently, entanglement entropy used for disordered interacting systems in equilibrium (Berkovits 2012, Franca et al 2013).

\[ \mathcal{E}_k = -2 \left( \frac{n_k}{2} - d_k \right) \log_2 \left( \frac{n_k}{2} - d_k \right) - d_k \log_2 d_k - (1 - n_k - d_k) \log_2 (1 - n_k - d_k) \]

Density in terms of \( G^< \), double occupancy via \( d_k = \frac{n_k^2}{4} + \frac{1}{U_k} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} \left( \Sigma_{MB}^< G^A + \Sigma_{MB}^R G^< \right)_{kk} \).

- For each set of parameters, we collect the pairs \( (n_k, \mathcal{E}_k) \) in a cumulative histogram
- In the non-interacting case, \( \mathcal{E}_k \) is completely determined by \( n_k \)
- On increasing \( U \), the spread of densities is reduced, and densities and entanglement are shifted to lower values.
- Increasing \( W \) increases the spread of the distributions, and a bias shifts the density to higher values.
- The variance of \( \mathcal{E}_k \) is smallest for \( U=2 \), corresponding to a crossover case the conductance.

Cumulative distribution of the single-site entanglement entropy \( \mathcal{E}_k \) as a function of the interaction strength for a 10-site chain with \( W = 2 \) and bias \( b_L = 0.5 \). The black solid curves at the base of the entanglement histograms correspond to \( \mathcal{E}_k \) for a non-interacting system, where \( n_k \in [0, 2] \) and \( \mathcal{E}_k \in [0, 2] \).
A possible connection between the non-monotonic behavior of current/conductance and entanglement, i.e. the latter could be an indicator of the competition between disorder and interactions.
Conclusions

Disorder vs Interactions
in systems out of equilibrium:

Competition & Crossover behavior

3D expanding fermionic clouds in optical lattices
- Multiple timescales in the melting of the Mott wedding-cake
- Disorder destabilizes the Mott plateau: dynamical crossover

1D disordered short Hubbard chains
- Enhancement of delocalization with a finite bias
- CPA treatment of disorder unsatisfactory
- Signatures of nonmonotonic behavior in the entanglement entropy
- Preliminary results from DFT provide additional perspective

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