Numerical renormalization group and multi-orbital Kondo physics

Theo Costi

Institute for Advanced Simulation (IAS-3) and
Institute for Theoretical Nanoelectronics (PGI-2)
Research Centre Jülich

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Autumn School on Correlated Electrons:
"From Kondo to Hubbard"

Outline

Collaborations

- Dr Hoa Nghiem (Postdoc, Juelich), Lukas Merker (PhD, Juelich)
- RWTH Aachen colaborators Dr Dante Kennes, Prof. Volker Meden (complementary methods, FRG/DMRG), Uni. Tuebingen, Prof. Sabine Andergassen (FRG)

References on NRG and codes

- K.G. Wilson, Rev. Mod. Phys. 1975 [Kondo model]
- Krishna-murthy et al, PRB 1980 [Anderson model]
- R. Bulla, T.A. Costi, T. Pruschke, Rev. Mod. Phys. 2008 [further developments/models]
- A. C. Hewson, The Kondo Problem to Heavy Fermions, C.U.P. (1997)
- Recommended public domain NRG codes:
  - "flexible DM-NRG" code (G. Zarand, et al., Budapest)
  - "NRG-Ljubljana" code (R. Zitko, Ljubljana)

Quantum impurity systems

- Impurity: small system, discrete spectrum
- Environment: large system, quasi-continuous spectrum
- Coupling: hybridization, Kondo exchange,...
- General structure:

$$H = H_{\text{imp}} + H_{\text{int}} + H_{\text{bath}}$$

Anderson model

- Single-level Anderson impurity model ($n_{d\sigma} = d_\sigma^\dagger d_\sigma$):

$$H_{AM} = \underbrace{\sum_\sigma \varepsilon_d n_{d\sigma} + U n_{d\uparrow} n_{d\downarrow}}_{H_{\text{imp}}} + \underbrace{\sum_{k\sigma} V_{kd}(c_{k\sigma}^\dagger d_\sigma + d_\sigma^\dagger c_{k\sigma})}_{H_{\text{int}}} + \underbrace{\sum_{k\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma}}_{H_{\text{bath}}} \quad (1)$$

- We take constant hybridization function:

$$\Delta(\omega) = \pi \sum_k V_{kd}^2 \delta(\omega - \epsilon_k) \approx \Delta(\epsilon_F = 0)$$

- non-constant hybridization can also be dealt with in NRG (e.g., for applications to DMFT, pseudogap systems,...)

Multi-orbital and multi-channel Anderson Model

- Rotationally symmetric case, e.g., for transition metal ions $l = 2$, and $m = -2, -1, 0, +1, +2$

$$H = \sum_{m\sigma} \varepsilon_{dm} n_{m\sigma} + \frac{1}{2} U \sum_{m\sigma} n_{m\sigma} n_{m-\sigma} + \frac{1}{2} U' \sum_{m\neq m'\sigma} n_{m\sigma} n_{m'-\sigma}$$

$$+\frac{1}{2}(U' - J) \sum_{m\neq m'\sigma} n_{m\sigma} n_{m'\sigma} - \frac{J}{2} \sum_{m\neq m'\sigma} d^{\dagger}_{m\sigma} d_{m-\sigma} d^{\dagger}_{m'-\sigma} d_{m'\sigma}$$

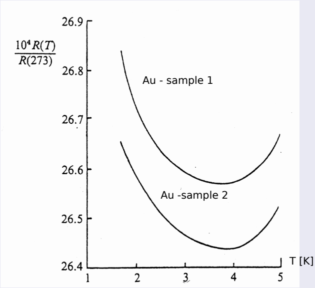
$$-\frac{J'}{2} \sum_{m\neq m'\sigma} d^{\dagger}_{m\sigma} d^{\dagger}_{m-\sigma} d_{m'-\sigma} d_{m'\sigma}$$

$$+\sum_{km\sigma} V_{km\sigma}(c^{\dagger}_{km\sigma} d_{m\sigma} + h.c.) + \sum_{km\sigma} \epsilon_{km\sigma} c^{\dagger}_{km\sigma} c_{km\sigma}$$

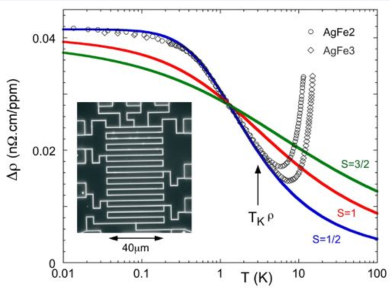
- Crystal field and spin-orbit interactions $\Rightarrow$
- Further lowering of symmetry, fewer channels

Magnetic impurities in non-magnetic metals

Fe in Au: de Haas et al 1934



Fe in Ag: Mallet et al 2006



- de Haas et al: resistivity minimum and increase as $T \to 0$!
- Kondo 1964: explanation in terms of magnetic impurities
- Kondo 1964: $R_{\mathrm{K}}(T) = -c_{\mathrm{imp}} \ln(k_{\mathrm{B}} T / D) \to \infty$ as $T \to 0$!!

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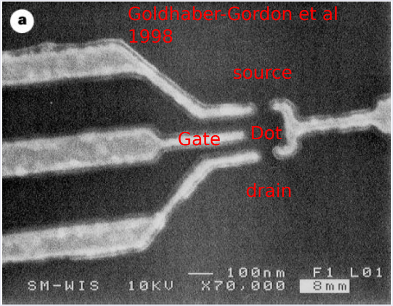
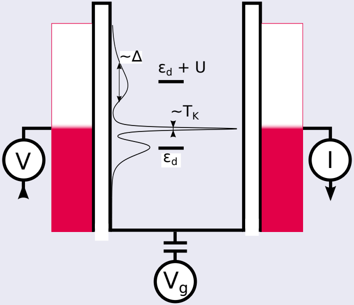
Quantum dots, Kondo effect and nanoscale size SET's

100nm lateral quantum dots



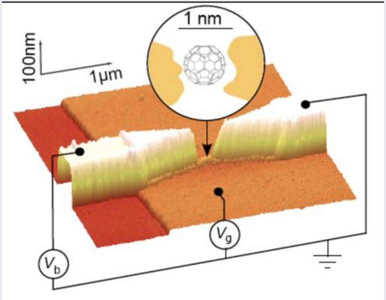
⇒ Tunable Kondo effect



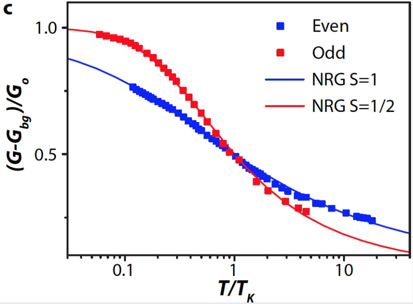
- $T_K = \sqrt{\Delta U/2} e^{\pi \varepsilon_d(\varepsilon_d + U)/2\Delta U}$ ⇒ exponential sensitivity
- Single-electron transistor based on Kondo effect

High/low spin molecules in nanogaps

C_{60}: Roch et al 2009



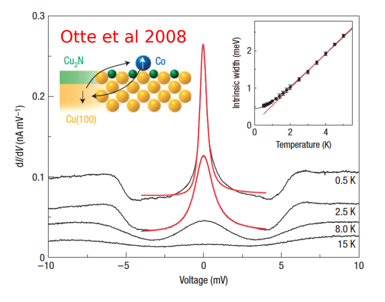
Underscreened Kondo effect



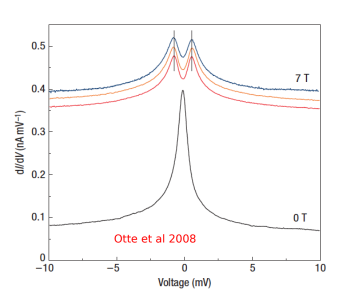
- Asymmetric lead couplings: partial screening of $S = 1 \Rightarrow$
- Underscreened Kondo effect (N. Roch et al PRL 2009)

Magnetic atoms on surfaces: Kondo + spin anisotropy

Co (S=3/2): Kondo+anisotropy



Ti (S=1/2): usual Kondo effect



- $H_{\rm imp} = -g\mu_B S_z + DS_z^2$ for Co adatom with S=3/2
- $D > 0 \Rightarrow m = 1/2 \leftrightarrow -1/2$ transitions $\Rightarrow$ Kondo effect
- $m = \pm 1/2 \rightarrow \pm 3/2$ transitions, side-bands to Kondo

NRG: linear chain form of the Anderson model

$$H_{AM} = \sum_{\sigma} \varepsilon_d n_{d\sigma} + U n_{d\uparrow} n_{d\downarrow} + \overbrace{V \sum_{\sigma} (f_{0\sigma}^\dagger d_\sigma + d_\sigma^\dagger f_{0\sigma})}^{V f_{0\sigma} = \sum_k V_{kd} c_{k\sigma}} + \sum_{k\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma}$$

Tridiagonalize $H_{\rm bath} = \sum_{k\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma}$ using Lanczos with starting vector defined by $V f_{0\sigma} = \sum_k V_{kd} c_{k\sigma}$ to obtain linear chain form:

$$H_{AM} = \sum_{\sigma} \varepsilon_d n_{d\sigma} + U n_{d\uparrow} n_{d\downarrow} + V \sum_{\sigma} (f_{0\sigma}^\dagger d_\sigma + d_\sigma^\dagger f_{0\sigma})$$
$$+ \sum_{n=0,\sigma}^{\infty} \epsilon_n f_{n\sigma}^{+} f_{n\sigma} + \sum_{n=0,\sigma}^{\infty} t_n (f_{n\sigma}^{+} f_{n+1\sigma} + H.c.)$$

...suitable for numerical treatment by adding one orbital at a time, starting with d_σ, then f_0, then f_1, ...

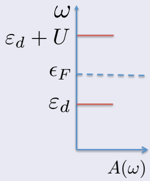
Atomic and zero-bandwidth limits

$$H_{AM}^{m=-1}(V=0) = \sum_{\sigma} \varepsilon_d n_{d\sigma} + U n_{d\uparrow} n_{d\downarrow}$$

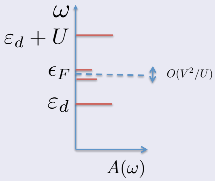
$$H_{AM}^{m=0}(\epsilon_k=0) = \sum_{\sigma} \varepsilon_d n_{d\sigma} + U n_{d\uparrow} n_{d\downarrow} + V \sum_{\sigma} (f_{0\sigma}^{\dagger} d_{\sigma} + d_{\sigma}^{\dagger} f_{0\sigma})$$

$$A_{\sigma}(\omega) = \frac{1}{Z} \sum_{p,q} |\langle p | d_{\sigma}^{\dagger} | q \rangle|^2 (e^{-\beta E_q} + e^{-\beta E_p}) \delta(\omega - (E_q - E_p))$$

$V=0$: atomic limit



$\epsilon_k = \epsilon_F = 0$: zero bandwidth limit



Anderson model: the Kondo resonance

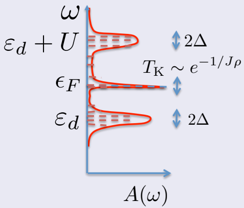
$$H_{AM} = \sum_{\sigma} \varepsilon_d n_{d\sigma} + U n_{d\uparrow} n_{d\downarrow} + V \sum_{k\sigma} (f^{\dagger}_{0\sigma} d_{\sigma} + d^{\dagger}_{\sigma} f_{0\sigma})$$

$$+ \sum_{n=0,\sigma}^{\infty} \epsilon_n f^{+}_{n\sigma} f_{n\sigma} + \sum_{n=0,\sigma}^{\infty} t_n (f^{+}_{n\sigma} f_{n+1\sigma} + H.c.)$$

Finite bandwidth

- Add $f_{1\sigma}, f_{2\sigma}, \ldots$
- $\Rightarrow$ broadening $O(\Delta)$ of ε_d, and $\varepsilon_d + U$ excitations
- $\Rightarrow$ Kondo resonance $T_{\mathrm{K}} \sim e^{-1/J\rho}, J \sim V^2/U$

Kondo resonance



Iterative diagonalization/recursion relation

- Define truncated Hamiltonian (m conduction orbitals):

$$H_{AM} \approx \quad H_m = \varepsilon_d n_d + U n_{d\uparrow} n_{d\downarrow} + V \sum_\sigma (f^+_{0\sigma} d_\sigma + d^+_\sigma f_{0\sigma})$$

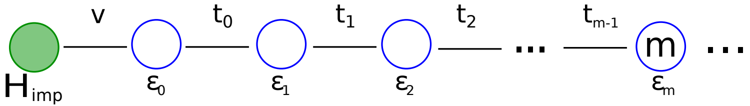
$$+ \quad \sum_{\sigma,n=0}^{m} \epsilon_n f^+_{n\sigma} f_{n\sigma} + \sum_{\sigma,n=0}^{m-1} t_n (f^+_{n\sigma} f_{n+1\sigma} + f^+_{n+1\sigma} f_{n\sigma})$$

- satisfying recursion relation:

$$H_{m+1} = H_m + \sum_\sigma \epsilon_{m+1} f^\dagger_{m+1\sigma} f_{m\sigma} + t_m \sum_\sigma (f^+_{m\sigma} f_{m+1\sigma} + f^+_{m+1\sigma} f_{m\sigma}).$$

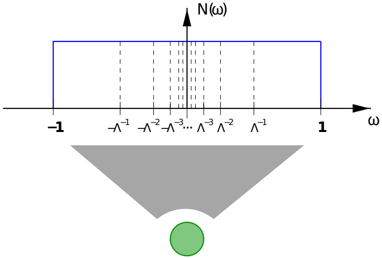
- diagonalize $H_m = \sum_p E^m_p |p\rangle_{m\,m}\langle p|$
- use product basis $|r, e_{m+1}\rangle \equiv |r\rangle_m |e_{m+1}\rangle$ with $|e_{m+1}\rangle = |0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle$ to set up matrix of H_{m+1} via recursion relation and diagonalize, ...

Iterative diagonalization



- Exact, if all states retained.
- In practice, no. states of H_m is $O(4^{m+1})$ ($= 4096$ at $m = 5$)
- Symmetries help $H_m = \sum \oplus H^m_{N_e,S,Sz}$
  $([\hat{N}_e, H_m] = [\vec{S}^2, H_m] = [S_z, H_m] = 0)$
- For $m > 5$, truncate to $O(1000)$ lowest eigenstates
- Truncation works, provided t_m decay sufficiently fast with m

Logarithmic discretization



- Logarithmic discretization of band $\epsilon_{k_n}/D = \pm\Lambda^{-n}, n = 0, 1, \ldots$ with $\Lambda > 1$, e.g. $\Lambda = 2$
- $\Rightarrow t_m \sim \Lambda^{-m/2}, \epsilon_m \sim \Lambda^{-m}$
- For $\Lambda \gg 1$, average over discretizations (Oliveira), $\epsilon_{k_n}/D = \pm\Lambda^{-n-z+1}, n = 1, \ldots (\pm 1, n = 0)$

NRG for multiple-channels

- Transition metal ions $l = 2$, and $m = -2, -1, 0, +1, +2$

$$H = H_{\rm imp}(\{\varepsilon_{dm}\}, U, U', J) + \sum_{km\sigma} \overbrace{V_{km}(c^\dagger_{km\sigma} d_{m\sigma} + h.c.)}^{V_m f_{0m\sigma} = \sum_k V_{km} c_{km\sigma}} + \sum_{km\sigma} \epsilon_{km\sigma} c^\dagger_{km\sigma} c_{km\sigma}$$

- Convert to linear chain form using Lanczos:

$$H = H_{\rm imp}(\{\varepsilon_{dm}\}, U, U', J) + \sum_{m\sigma} V_m(f_{0m\sigma} d_{m\sigma} + h.c.) + \sum_{n=0}^{+\infty} \sum_{m\sigma} \epsilon_{nm} f^\dagger_{nm\sigma} f_{nm\sigma} + \sum_{n=0}^{+\infty} \sum_{m\sigma} t_{nm}(f^\dagger_{nm\sigma} f_{n+1m\sigma} + h.c.)$$

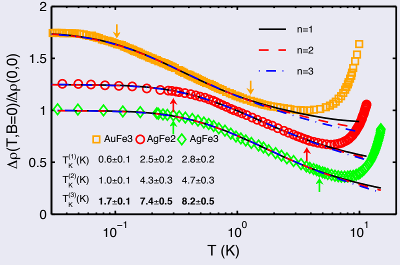
- NRG: Hilbert space increases by $4^{2l+1} = 1024$ per shell added !

NRG for multiple-channels: exploiting symmetries

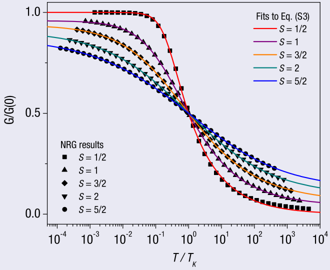
- For 3-channel $S = 3/2$ Kondo model, without symmetries, fraction of kept states $= 1/4^3 = 1/64$.
- implementing $SU(3)$ symmetries (Hanl, Weichselbaum et al, PRB 2013) increased this fraction to $\approx 1/4^2 = 1/16$, making the 3-channel Kondo calculation equivalent to a 2-channel calculation
- allowed comparing to experimental resistivity ($R(T)$) and dephasing ($\tau_\varphi(T)$) data for Fe/Au for

Multi-channel fully screened/single-channel underscreened resistivities

Resistivity for 3 channel $S = 3/2$ Kondo model, Hanl et al PRB 2013

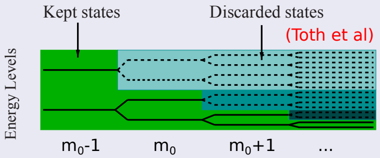


Resistivity for 1-channel spin $S \geq 1/2$ Kondo model, Parks et al Science 2010



Output from NRG procedure

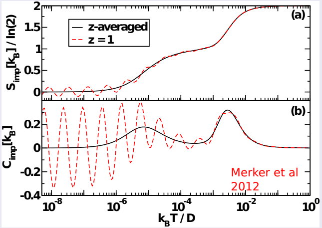
Kept/discarded states



- Many-body eigenvalues E_p^m and eigenvectors $|p\rangle_m$ on all relevant energy scales $t_m \sim \Lambda^{-m/2}$, $m = 0, 1, ..., N$.
- From eigenvalues calculate $Z = \sum_p e^{-\beta E_p}$ and thermodynamics
- From eigenstates calculate matrix elements, hence Green functions and transport
- Discarded states not used in iterative diagonalization, but useful for calculating physical properties (see later)

Thermodynamics

Impurity entropy/specific heat



- Entropy

$$S(T) = (E - F)/T,$$
$$E = \langle H_{AM} \rangle,$$
$$F = -\frac{1}{\beta} \ln Z$$

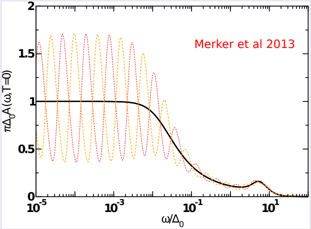
- Specific heat

$$C(T) = k_\mathrm{B} \beta^2 \langle H_{AM}^2 - \langle H_{AM} \rangle^2 \rangle$$

- Discretization oscillations at $\Lambda \gg 1$ eliminated by z-averaging (here $\Lambda = 4$, $n_z = 2$).

Dynamics

d-spectral function



- NRG spectra are discrete ($\Delta E_{qq'} = E_{q'} - E_q$):

$$A_{d\sigma}(\omega, T) = \sum_{q,q'} w_{qq'}(T)\delta\left(\omega - \Delta E_{qq'}\right)$$

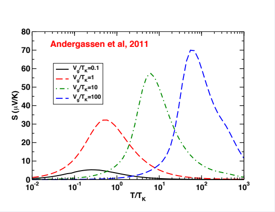
- broaden with logarithmic Gaussians:

$$\delta(\omega - \Delta E_{q'q}) \rightarrow \frac{e^{-b^2/4}}{b|\Delta E_{q'q}|\sqrt{\pi}} e^{-(ln(\omega/\Delta E_{q'q})/b)^2}$$

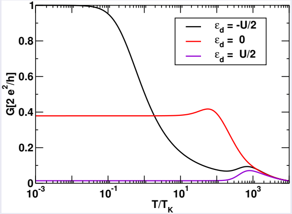
- Discretization oscillations at $\Lambda \gg 1$ eliminated by z-averaging (here $\Lambda = 10$, $n_z = 8$).

Linear transport

Thermopower for $U < 0$



Conductance: Merker et al



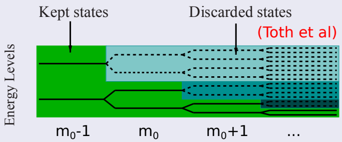
- Linear response transport from spectral functions $A(\omega, T)$:

$$G(T) = \frac{e^2}{h} \int d\omega \left(-\frac{\partial f}{\partial \omega} \right) \sum_\sigma \overbrace{\mathcal{T}_\sigma(\omega, T)}^{\propto A(\omega, T)},$$

$$S(T) = -\frac{1}{|e|T} \frac{\int d\omega \, \omega \, (-\partial f / \partial \omega) \sum_\sigma \mathcal{T}_\sigma(\omega, T)}{\int d\omega \, (-\partial f / \partial \omega) \sum_\sigma \mathcal{T}_\sigma(\omega, T)}$$

Kept states in NRG

Kept/discarded states



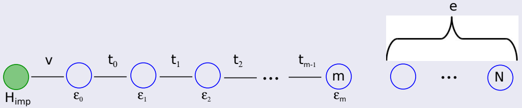
$Z = \sum_p e^{-\beta E_p}$

- $Z \neq \sum_{m=0}^{N} \overbrace{\sum_p e^{-\beta E_p^m}}^{=Z_m(T)}$
- Double counting
- Conventional approach: $Z(T) \approx Z_m(T)$ for $T \equiv T_m \sim t_m$

- Use discarded states to build a complete set of eigenstates for summing up unambiguously contributions from different H_m (Anders & Schiller 2005)
- All states must reside in same Hilbert space: that of H_N

Construction of the complete basis set

Environment states



- $H_m|qm\rangle = E_q^m|qm\rangle$, $q = (k, l) = ($kept,discarded$)$
- Product states $|lem\rangle = |lm\rangle \otimes |e\rangle$ with $e = (e_{m+1}, ..., e_N\rangle$, $m = m_0, ..., N$ form a complete set (Anders & Schiller 2005)

$$\sum_{m=m_0}^{N} \sum_{le} |lem\rangle\langle lem| = 1$$

- Allows unambiguous summation of contributions from different H_m

Full density matrix (FDM)

- Full density matrix and partition function (Weichselbaum & von Delft 2007):

$$\rho = \frac{1}{Z(T)} \sum_{m=m_0}^{N} \sum_{le} e^{-\beta E_l^m} |lem\rangle\langle lem|, \quad \mathrm{Tr}\rho = 1 \Rightarrow$$

$$Z(T) = \sum_{m=m_0}^{N} 4^{N-m} \sum_{l} e^{-\beta E_l^m} \equiv \sum_{m=m_0}^{N} 4^{N-m} Z_m(T)$$

- Rewrite ρ as weighted sum of shell density matrices $\tilde{\rho}_m$:

$$\rho = \sum_{m=m_0}^{N} w_m \tilde{\rho}_m, \quad \tilde{\rho}_m = \sum_{le} |lem\rangle \frac{e^{-\beta E_l^m}}{\tilde{Z}_m} \langle lem|.$$

$$Tr\,[\tilde{\rho}_m] = 1, \quad w_m = 4^{N-m}\frac{Z_m}{Z}, \quad \sum_{m=m_0}^{N} w_m = 1$$

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Thermodynamics

- Local observables $\hat{O} = n_d, \quad n_{d\uparrow} n_{d\downarrow}, \quad d^\dagger_\sigma f_{0\sigma}, \quad S_z, \ldots$

$$\langle \hat{O} \rangle_\rho = \mathrm{Tr}\left[\rho \hat{O}\right] = \sum_{l'e'm'} \langle l'e'm' | \rho \hat{O} | l'e'm' \rangle$$

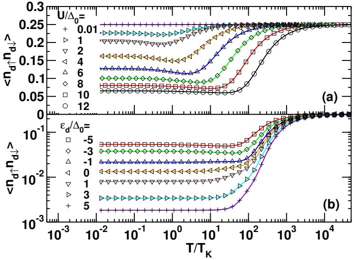
$$= \sum_{l'e'm'} \sum_{lem} w_m \overbrace{\langle l'e'm' | lem \rangle}^{\delta_{ll'ee'mm'}} \frac{e^{-\beta E_l^m}}{\tilde{Z}_m} \overbrace{\langle lem | \hat{O} | l'e'm' \rangle}^{O_{ll}^m}$$

$$= \sum_{lem} w_m \frac{e^{-\beta E_l^m}}{\tilde{Z}_m} O_{ll}^m = \sum_{lm} 4^{N-m} w_m O_{ll}^m \frac{e^{-\beta E_l^m}}{4^{N-m} Z_m}$$

$$= \sum_{m=m_0,l}^{N} w_m O_{ll}^m \frac{e^{-\beta E_l^m}}{Z_m}$$

Double occupancy

- Double occupancy: $\langle n_{d\uparrow} n_{d\downarrow} \rangle \rightarrow \langle n_{d\uparrow} \rangle \langle n_{d\downarrow} \rangle, U \rightarrow 0$
- Double occupancy: $\langle n_{d\uparrow} n_{d\downarrow} \rangle \ll 1, U \gg \Delta$
- FDM (lines) and conventional (symbols) in excellent agreement: FDM simpler, obviates need to chose best shell for given T



Dynamics

- Evaluation of equilibrium retarded Green function (Weichselbaum & von Delft 2007; Peters et al 2006):

$$G_{AB}(t) = -i\theta(t)\langle[A(t), B]_{+}\rangle \equiv -i\theta(t)\mathrm{Tr}\left[\rho(A(t)B + BA(t))\right]$$
$$= -i\theta(t)\left[C_{A(t)B} + C_{BA(t)}\right]$$

- Consider correlation function $C_{A(t)B}$:

$$C_{A(t)B} = \mathrm{Tr}\left[\rho A(t)B\right] = \mathrm{Tr}\left[\rho A(t)B\right] = \mathrm{Tr}\left[\rho A(t)\hat{1}B\right]$$
$$= \sum_{lem}\langle lem|e^{-iHt}Ae^{iHt}\sum_{l'e'm'}|l'e'm'\rangle\langle l'e'm'|B\rho|lem\rangle$$
$$= \sum_{lem}\sum_{l'e'm'}\underbrace{\langle lem|e^{-iHt}Ae^{iHt}|l'e'm'\rangle}_{e^{i(E^{m'}_{l'}-E^{m}_{l})t}\langle l'e'm'|A|lem\rangle}\langle l'e'm'|B\rho|lem\rangle$$

Dynamics

- ... Peters et al 2006

$$C_{A(t)B}^{m'>m} = \sum_{lem} \langle lem | e^{-iHt} A e^{iHt} \overbrace{\sum_{l'e'm'>m} |l'e'm'\rangle\langle l'e'm'|}^{=|kem\rangle\langle kem|} B\rho | lem\rangle$$

- Avoid off-diagonal matrix elements $A_{ll'}^{m\neq m'}$ by using

$$1 = 1_m^- + 1_m^+$$

$$1_m^- = \sum_{m'=m_0}^{m} \sum_{l'e'} |l'e'm'\rangle\langle l'e'm'|$$

$$1_m^+ = \sum_{m'=m+1}^{N} \sum_{l'e'} |l'e'm'\rangle\langle l'e'm'| = \sum_{ke} |kem\rangle\langle kem|.$$

Dynamics

- ... only shell diagonal matrix elements appear: $A^m_{ll'}$
- ... and reduced density matrices Hofstetter 2000:
  $R^m_{\mathrm{red}}(k',k) = \sum_e \langle k'em|\rho|kem\rangle$

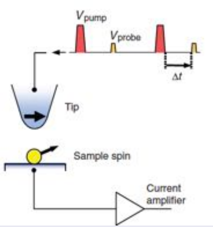
$$G_{AB}(\omega + i\delta) = \sum_m \frac{w_m}{Z_m} \sum_{ll'} A^m_{ll'} B^m_{l'l} \frac{e^{-\beta E^m_l} + e^{-\beta E^m_{l'}}}{\omega + i\delta - (E^m_{l'} - E^m_l)}$$

$$+ \sum_m \frac{w_m}{Z_m} \sum_{lk} A^m_{lk} B^m_{kl} \frac{e^{-\beta E^m_l}}{\omega + i\delta - (E^m_k - E^m_l)} + \ldots$$

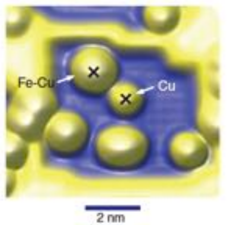
$$+ \sum_m \sum_{lkk'} A^m_{kl} B^m_{lk'} \frac{R^m_{\mathrm{red}}(k',k)}{\omega + i\delta - (E^m_l - E^m_k)} + \ldots$$

Motivation: pump-probe spectroscopies

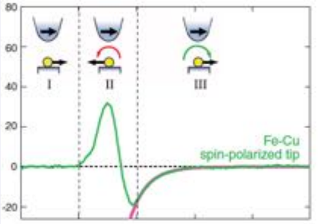
Loth et al 2010



Fe on CuN/Cu



Spin relaxation



Transient response following a sudden quench

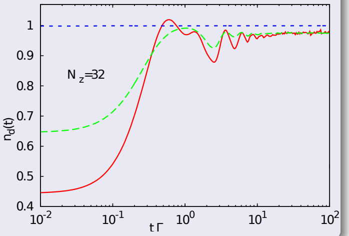
$H(t) = \theta(-t)H^i + \theta(t)H^f$

$$O(t) = Tr\left[e^{-iH^f t}\rho e^{iH^f t}\hat{O}\right]$$

$$= \sum_{m=m_0}^{N} \sum_{rs \notin KK'} \rho_{sr}^{i\to f}(m) e^{-i(E_s^m - E_r^m)t} O_{rs}^m$$

(Anders & Schiller 2005
FDM gen.: Nghiem & Costi 2014)

$\varepsilon_d(t) = -\theta(t)U/2$:
Nghiem et al 2014



- $O(t \to 0^+)$ exact in TDNRG (Nghiem et al PRB 2014)
- $O(t \to \infty)$ not exact in TDNRG (Anders & Schiller 2005, Nghiem et al PRB 2014)

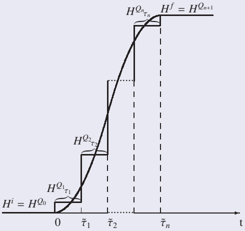
Multiple quenches and general pulses

n-Quantum quenches

$$\rho(t) = e^{-iH^{Q_{p+1}}(t-\tilde{\tau}_p)} e^{-iH^{Q_p}\tau_p} \ldots e^{-iH^{Q_1}\tau_1} \rho$$
$$\times\, e^{iH^{Q_1}\tau_1} \ldots e^{iH^{Q_p}\tau_p} e^{iH^{Q_{p+1}}(t-\tilde{\tau}_p)}$$

$$O(t) = Tr\left[e^{-iH^f t} \rho e^{iH^f t} \hat{O}\right]$$
$$= \sum_{mrs}^{\notin KK'} \rho_{rs}^{i\to Q_{p+1}}(m, \tilde{\tau}_p) e^{-i(E_r^m - E_s^m)(t-\tilde{\tau}_p)} O_{sr}^m$$

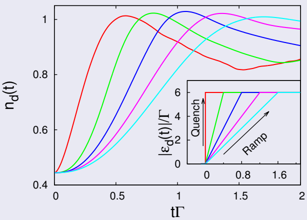
Nghiem et al 2014



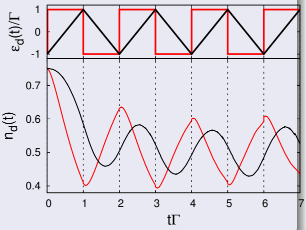
- Formalism rests ONLY on NRG (truncation) approximation!
- Other approaches use hybrid (DMRG-TDNRG) and additional approximations (Eidelstein et al 2013)

General pulses and periodic switching

linear ramp: Nghiem & Costi 2014



periodic switching



- Linear ramp: time-delay in occupation $n_d(t)$
- Periodic switching ($U = 0$): coherent control of nanodevices (qubits,...)

Summary

- NRG: powerful method for strongly correlated systems
- NRG: still in development for:
  - time-dependent & non-equilibrium phenomena
  - complex multi-channel models (see Mitchell et al PRB 2013)
- Plenty of work still to do for smart PhD students !