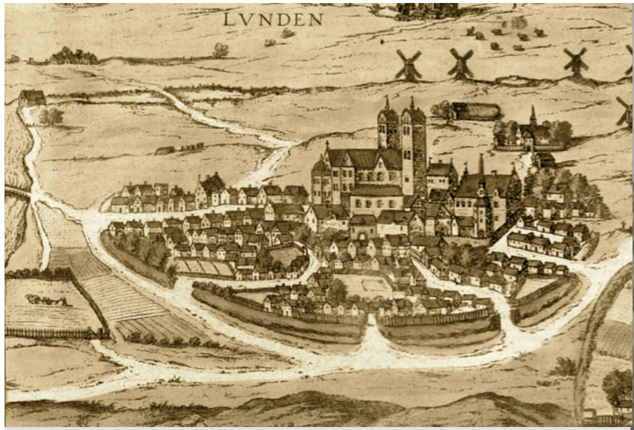

Steering Magnetic Skyrmions with NEGF

What about localized spins ?

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KBEt^2 *Kiel 12^h March 2019*

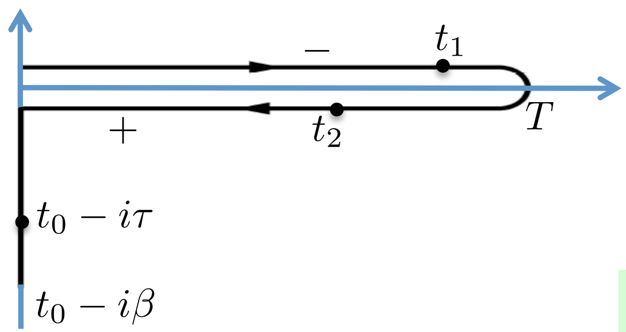
Kadanoff-Baym Equations (KBE)

Basic quantity

$$G(1,1') = \frac{1}{i} \frac{\mathrm{Tr}\left[\mathcal{T}_\gamma\{e^{-i\int_\gamma d\bar{z}\hat{H}(\bar{z})}\hat{\psi}(\mathbf{x}_1,z_1)\hat{\psi}^\dagger(\mathbf{x}_1',z_1')\}\right]}{\mathrm{Tr}\left[\mathcal{T}_\gamma\{e^{-i\int_\gamma d\bar{z}\hat{H}(\bar{z})}\}\right]}$$

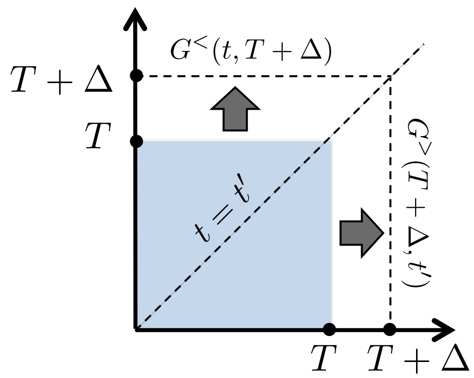
Basic equation

$$[i\partial_{t_1} - h(t_1)]G(t_1,t_2) = \delta(t_1,t_2) + \int_\gamma dt\, \Sigma(t_1,t)G(t,t_2)$$



$$\Sigma(1,2) = \frac{\delta\Phi[G]}{\delta G(2,1)}$$

problem scales as N^3



Some references on NEGF/GKBA+MBA

Kadanoff and Baym (1962); Keldysh, JETP (1965); Danielewicz (1984); Lipavsky, Spicka and B. Velicky (1986), Jauho et al (1994); Kohler et al (1999); Kwong and Bonitz (2000); Semkat, Bonitz and Kremp (2003); Stefanucci and Almbladh (2004); Dahlen van Leeuwen (2006)); Fransson (2008); Myhöhänen et al., (2008); Puig, Verdozzi, Almbladh (2009); Balzer, Bonitz et al, (2010) ; Tuovinen et al (2013); Latini et al (2014); Hermanns et al (2014); Perfetto et al (2015); Sangalli and Marini (2015); Melo and Marini (2015); Ridley et al (2015); N. Schlünzen et al (2016); Hopjan et al (2016); Schüler, Berakdar, and Pavlyukh (2016); Covito et al (2018); Mahzoon, P Danielewicz, A Rios (2018); Hopjan and Verdozzi (2018)); Karlsson et al (2018); Bonitz et al (2018).

Books: see e.g.

Jauho Fransson (2010); K. Balzer and M. Bonitz's, Springer (2013), Kamenev ambridge Univ. Press (2012), Stefanucci and van Leeuwen, Cambridge Univ. Press (2013)

GENERALIZED KADANOFF-BAYM ANSATZ (GKBA): $N^3 \rightarrow N^2$

$$G(1,2) = \theta(t_1,t_2)G^>(1,2) + \theta(t_2,t_1)G^<(1,2)$$

$$\left[i\frac{d}{dt} - h_{\mathrm{HF}}(t)\right] G^<(t,t') = I^<(t,t')$$

$$I^<(t,t') = \int_{-\infty}^{\infty} d\bar{t}\left[\Sigma^<(t,\bar{t})G^{\mathrm{A}}(\bar{t},t') + \Sigma^{\mathrm{R}}(t,\bar{t})G^<(\bar{t},t')\right]$$

Subtracting the adjoint $$\frac{d}{dt}\rho(t) + i\left[h_{\mathrm{HF}}(t),\rho(t)\right] = -\left(I^<(t,t) + \mathrm{H.c.}\right).$$

Because of $G^<$, not a closed equation for ρ.

$$G^<(t,t') = -G^{\mathrm{R}}(t,t')\rho(t') + \rho(t)G^{\mathrm{A}}(t,t')$$

$$G^>(t,t') = G^{\mathrm{R}}(t,t')\bar{\rho}(t') - \bar{\rho}(t)G^{\mathrm{A}}(t,t')$$

$$\rho(t) = -iG^<(t,t) \quad \bar{\rho}(t) = 1-\rho(t) = iG^>(t,t)$$

$$G^{\mathrm{R}} - G^{\mathrm{A}} = G^> - G^<$$

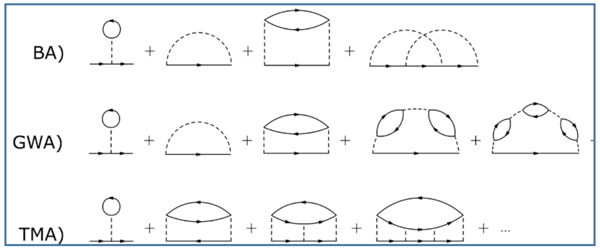
Possible choice: $$G^{\mathrm{R/A}}(t,t') = \mp i\theta[\pm(t-t')]Te^{-i\int_{t'}^{t} d\bar{t}\ h_{HF}(\bar{t})}$$

GKBA initial correlated states: via adiabatic ramping of interactions

We use/adapt an early version of the CHEERS code

NEGF and Many-Body Approximations

Some Many Body Approximations



$$\Sigma_{TMA}(12) = \Sigma_{HF} + iU^2 G(21)T(12)$$

$$T = \phi - \phi \mathcal{U} T, \quad \phi(12) = -iG(12)G(12)$$

Ehrenfest approximation (EA)

$$H_n = \sum_\nu \frac{p_\nu^2}{2M_\nu} + U_{cl}(\mathbf{x})$$

$$i\frac{d}{dt}|\psi(t)\rangle = \hat{H}_e(\mathbf{x}(t),t)|\psi(t)\rangle$$

$$\frac{dp_\nu}{dt} = -\frac{\partial}{\partial x_\nu}[U_{cl}(\mathbf{x}(t)) + \langle\psi(t)|\hat{H}_e(\mathbf{x}(t),t)|\psi(t)\rangle]$$

A quantum / classical scheme
In connection with NEGF, introduced in

Balzer, Schlünzen, Bonitz, Phys. Rev. B 94, 245118 (2016)
Boström, Hopjan, Kartsev, Verdozzi, Almbladh, J. Phys.: Conf. Ser. 696, 2016)

Here: EA for spin dynamics

see also works from M. Potthoff, B. Nikolic, J. Fransson

Why Skyrmions ?

Vortex-like magnetic configurations/quasiparticles.

Chiral/achiral excited/(meta)stable states

Topological notion:

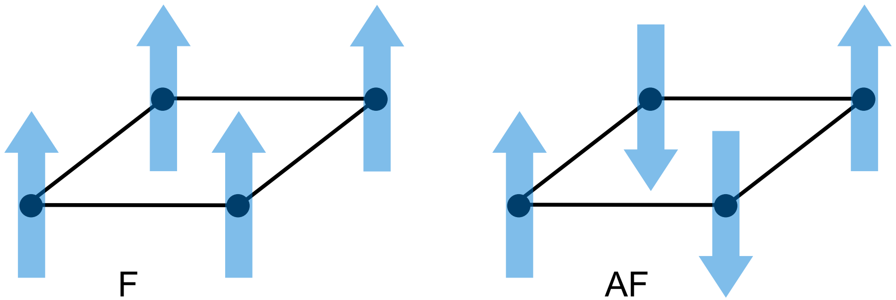
integer topological index/charge/quantum number, skyrmion number

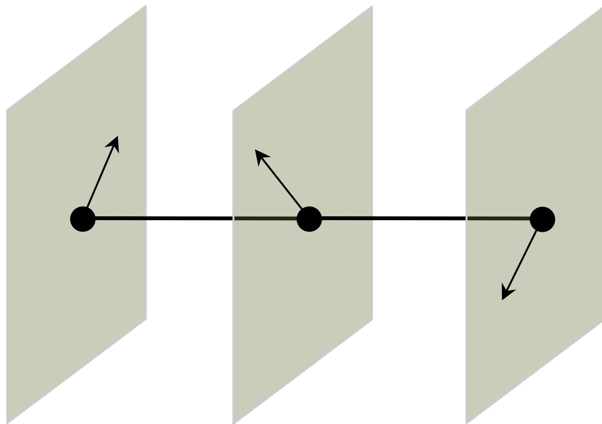
Spins all orthonormal to a film plane, except for a region: spins progressively turn to anti-parallel, free energy minimized by circular symmetry

- Discrete magnetic states to store information:
- Skyrmion (logical 1) vs ferromagnetic (logical 0)
- Position manipulated with spin currents/waves

Spin Hamiltonian

Dzyaloshinskii-Moriya interaction
- Anti-symmetric exchange between neighboring spins
- Super-exchange from spin-orbit coupling
- Favors spin canting of otherwise (anti-) parallel moments





$J \gg D$
Magnetic ordering

$D \gg J$
Spiral ordering

The system

$$H = H_S + H_e + H_{S-e}$$

SPINS

$$\hat{\mathbf{e}}_{mn} \equiv \frac{\mathbf{R}_m - \mathbf{R}_n}{|\mathbf{R}_m - \mathbf{R}_n|}$$

$$H_S = -J \sum_{mn} \mathbf{S}_m \cdot \mathbf{S}_n - D \sum_{mn} \hat{\mathbf{e}}_{mn} \cdot (\mathbf{S}_m \times \mathbf{S}_n) - h(t) \sum_m S_m^z$$
$$+ A_1 \sum_m \sum_{i=x,y,z} (\hat{S}_m^i)^4 - A_2 \sum_{\langle mn \rangle} [\hat{S}_m^x \hat{S}_n^x + \hat{S}_m^y \hat{S}_n^y]$$

WIRE

spin-orbit

$$H_e = \sum_{i\sigma\sigma'} c_{i\sigma}^\dagger (\epsilon_i \hat{I} - h(t)\sigma_z)_{\sigma\sigma'} c_{i\sigma'} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \sum_{i\sigma\sigma'} \left[c_{i\sigma}^\dagger (t\hat{I} + it_{so}\sigma_y)_{\sigma\sigma'} c_{i+1,\sigma'} + h.c. \right]$$
$$+ t' \sum_{i\sigma\alpha} (a_{i\sigma\alpha}^\dagger a_{i+1,\sigma\alpha} + h.c.) + \sum_{i\sigma\alpha} u_\alpha(t) n_{i\sigma\alpha} + t_l \sum_\sigma (a_{1\sigma l}^\dagger c_{1,\sigma} + h.c.) + t_r \sum_\sigma (a_{1\sigma r}^\dagger c_{N,\sigma} + h.c.)$$

INTERACTION

$$H_{S-e} = J' \sum_i \mathbf{S}_i \cdot \sum_{\sigma\sigma'} c_{i\sigma}^\dagger \boldsymbol{\sigma}_{\sigma\sigma'} c_{i\sigma}$$

H_S from Yi, Nagaosa, and Han, PRB 80, 054416 (2009)

Treatment

a) MC for spins

b) contact electrons (in nanowire without leads) and spins:

$$\mathbf{F}_{m,G} = \alpha_G \mathbf{S}_m \times \left(\frac{\partial \mathbf{S}_m}{\partial t} \right)$$

HF for electrons with damped dynamics and pred.-corr. scheme

1. Calculate the electronic potential generated by the spins via $J' \sum_i \mathbf{S}_i \cdot \sum_{\sigma\sigma'} c^\dagger_{i\sigma} \boldsymbol{\sigma}_{\sigma\sigma'} c_{i\sigma}$

2. Calculate spin forces

$$\frac{\partial \mathbf{S}_m}{\partial t} = -2J \sum_n \mathbf{S}_n \times \mathbf{S}_m - \mathbf{h}(t) \times \mathbf{S}_m - 2D \sum_n [\hat{\mathbf{e}}_{mn}(\mathbf{S}_m \cdot \mathbf{S}_n) - (\hat{\mathbf{e}}_{mn} \cdot \mathbf{S}_m)\mathbf{S}_n] + 4A_1 \mathbf{A}_m \times \mathbf{S}_m + A_2 \mathbf{B}_m \times \mathbf{S}_m - \sum_{i\sigma\sigma'} J'_{im} \rho_{i\sigma,i\sigma'} (\boldsymbol{\sigma}_{\sigma\sigma'} \times \mathbf{S}_m),$$

$$\mathbf{A}_m = ([S^x_m]^3, [S^y_m]^3, [S^z_m]^3)$$
$$\mathbf{B}_m = (S_{m+\hat{\mathbf{x}}}, S_{m+\hat{\mathbf{y}}}, 0)$$

3. Find the Hartree-Fock ground state of the electrons

4. Update classical spins

5. Repeat until force on spins below threshold value

Treatment

c) ramping lead and e-e interactions (2nd Born): ramping in GKBA for non-collinear spins

d) Time evolution

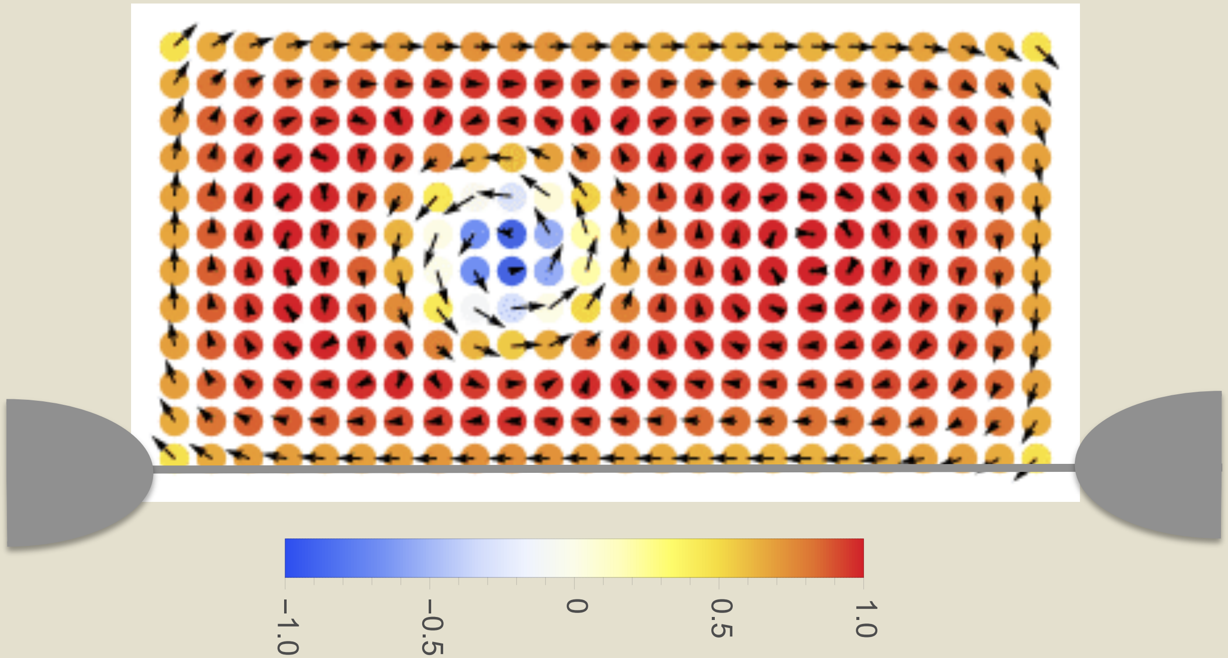
$$\frac{\partial}{\partial t}\rho(t) + i[h_{HF}(\{\mathbf{S}_n(t)\}, t), \rho(t)] = -(I^<(t,t) + h.c.),$$

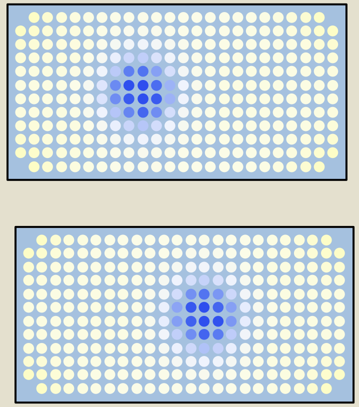
$$\rho_{i\sigma,j\sigma'} \equiv \begin{pmatrix} \rho_{\uparrow\uparrow} & \rho_{\uparrow\downarrow} \\ \rho_{\downarrow\uparrow} & \rho_{\downarrow\downarrow} \end{pmatrix}$$

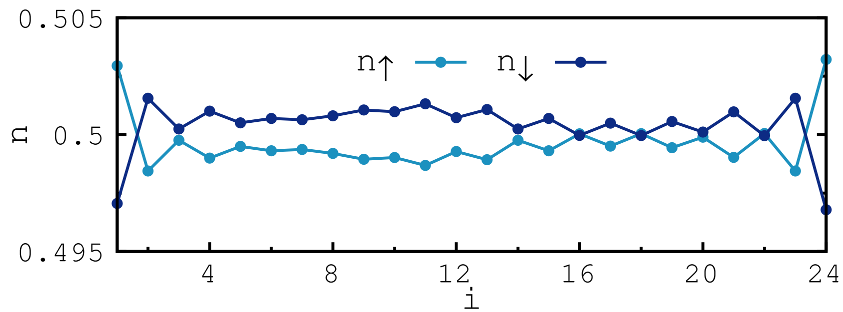
Leads fully spin-polarized.
Wire connected to 2 left/right leads (spin up/down) for spin currents

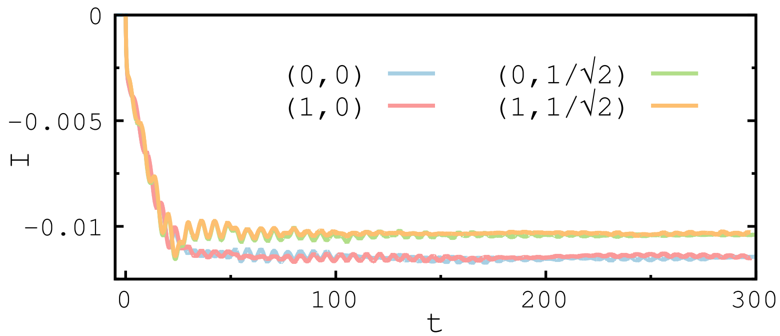
Steering a small skyrmion

1) Sudden switch-on of the bias
2) Leads fully spin-polarized
3) U=0
4) No SO







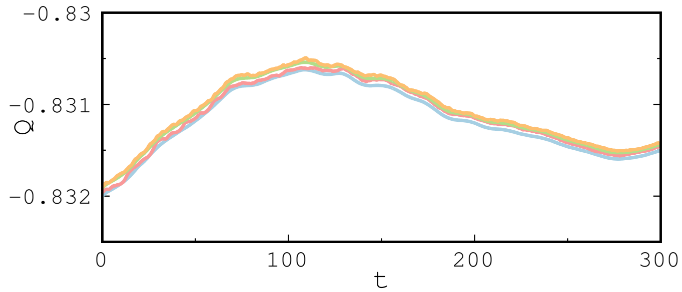


Characterizing the skyrmion motion

$$\varrho^{\mathcal{SK}} = \frac{1}{4\pi} \int \mathbf{M} \cdot \left(\frac{\partial \mathbf{M}}{\partial x} \times \frac{\partial \mathbf{M}}{\partial y} \right) dxdy$$

charge

$$Q(t) = \sum_m \varrho_m^{\mathcal{SK}}(t).$$

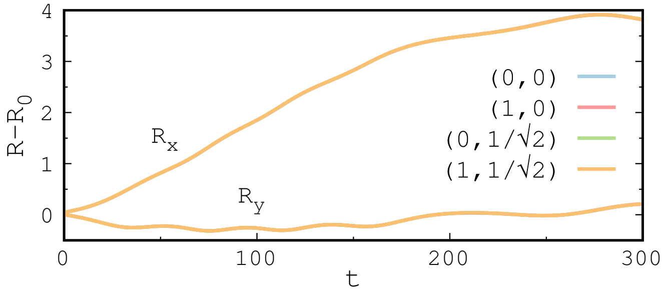


In extended lattice or periodic BC, Q is integer. However, for a finite system with fixed BC, Q can be no longer perfectly quantized,

Results support skyrmion rigid motion

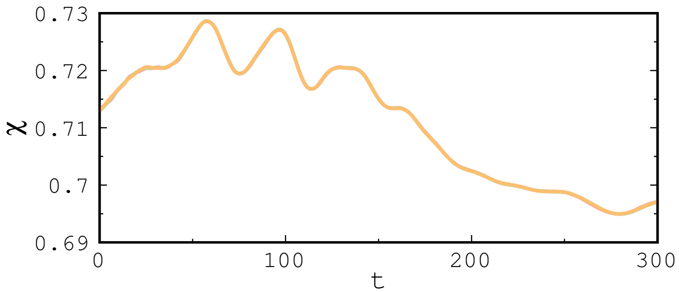
center of mass

$$\mathbf{R}(t) = \frac{\sum_m |\varrho_m^{\mathcal{SK}}(t)| \mathbf{R}_m}{\sum_m |\varrho_m^{\mathcal{SK}}(t)|}.$$



IPR

$$\chi(t) \equiv \frac{\sum_m |\varrho_m^{\mathcal{SK}}(t)|^2}{\left[\sum_m |\varrho_m^{\mathcal{SK}}(t)|\right]^2}.$$



Want to look at

- *optimally controlled dynamics; role of e-e interactions, spin-orbits, disorder, pressure*

Hurdle ahead: Size/time and quantum effects

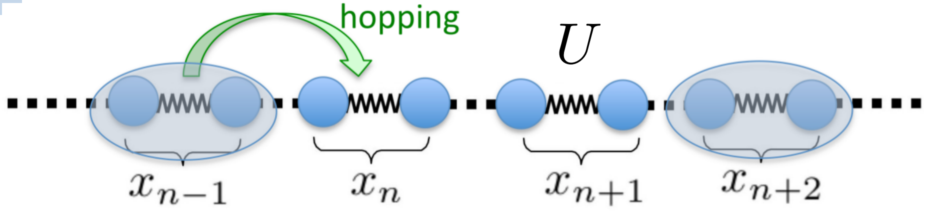
- The size of a skirmion
- Many skyrmions
- Manipulation of skyrmions with electronic circuitry

1) Remove e-e interactions: (e. g. Nikolic et al)

2) For classical spins, integrate out electronic degrees of freedom (e.g. Fransson et al, Potthoff et al, Ebert et al for spins, Hopjan et al for nuclei) a two component hybrid method for spins + electrons ?

Insight from the Hubbard-Holstein model

The Hubbard-Holstein model



$$\hat{H} = \sum_{i\sigma}(v_i - \mu)\hat{n}_{i\sigma} + U\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} - J\sum_{\langle ij\rangle\sigma} c^\dagger_{i\sigma}c_{j\sigma} + \omega\sum_i b^\dagger_i b_i + \sum_i \sqrt{2}\eta_i\,\hat{x}_i + \sqrt{2}g\sum_i(\hat{n}_{i\uparrow}+\hat{n}_{i\downarrow}-1)\hat{x}_i$$

$$\hat{x}_i = (b^\dagger_i + b_i)/2,\;\; \hat{p}_i = i(b^\dagger_i - b_i)/2$$

Lang-Firsov transformation necessary for DMFT solution

$$\tilde{H} = e^{iS}He^{-iS}$$

$$S = \frac{\sqrt{2}}{\omega_0}\sum_i \hat{p}_i(g(\hat{n}_i - 1) + \eta)$$

Renormalized parameters

$$v' = v + (g^2 - 2g\eta)/\omega$$

$$U' = U - 2g^2/\omega$$

$$\hat{t}'_{ij} = te^{i\sqrt{2}g(\hat{p}_i - \hat{p}_j)/\omega}$$

$$H' = \sum_{i\sigma}(v' - \mu)\hat{n}_{i\sigma} + \sum_i U'\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} - \sum_{\langle ij\rangle\sigma}\left(\hat{t}'_{ij}c^\dagger_{i\sigma}c_{j\sigma} + h.c.\right) + \sum_i\left[\omega b^\dagger_i b_i - \frac{(\eta - g)^2}{\omega}\right]$$

DFT of the HH model

E. Viñas Boström, P. Helmer, P. Werner, C. Verdozzi

Hohenberg-Kohn theorem
A one-to-one mapping $(\mu, \eta) \leftrightarrow (n, x)$

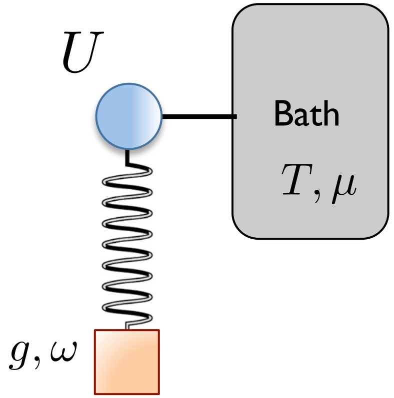
Kohn-Sham construction
Non-interacting system reproduces (n, x)

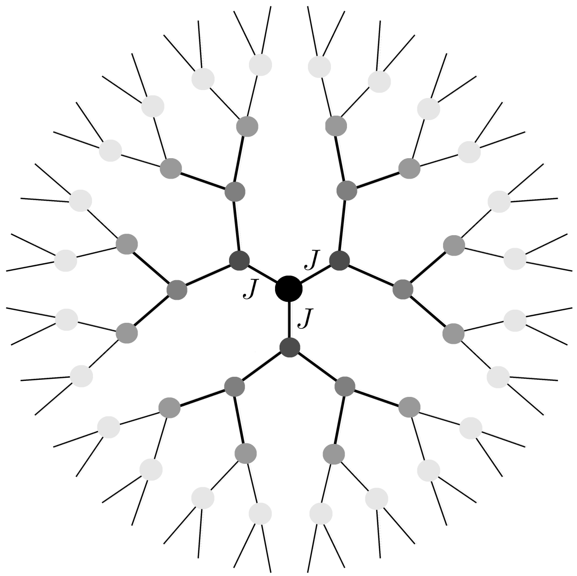
$$H_s^{(e)} = (v_{KS}[n,x] - \mu) \sum_{i\sigma} \hat{n}_{i\sigma} - \sum_{\langle ij \rangle \sigma} J \left(c_{i\sigma}^\dagger c_{j\sigma} + h.c. \right),$$

$$H_s^{(ph)} = \omega \sum_i b_i^\dagger b_i + \sqrt{2} \eta_{KS}[n,x] \sum_i \hat{x}_i \ .$$

Solve single HH site and Bethe's lattice Gives total energy → potentials

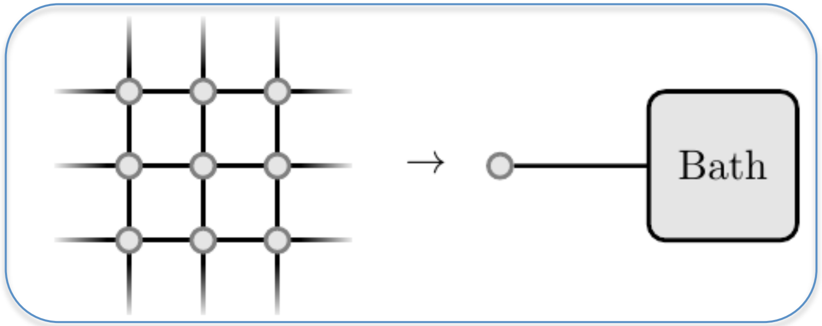
Analytical Solution





DMFT

HH model in D = ∞: DMFT-DFT results for v_{xc}



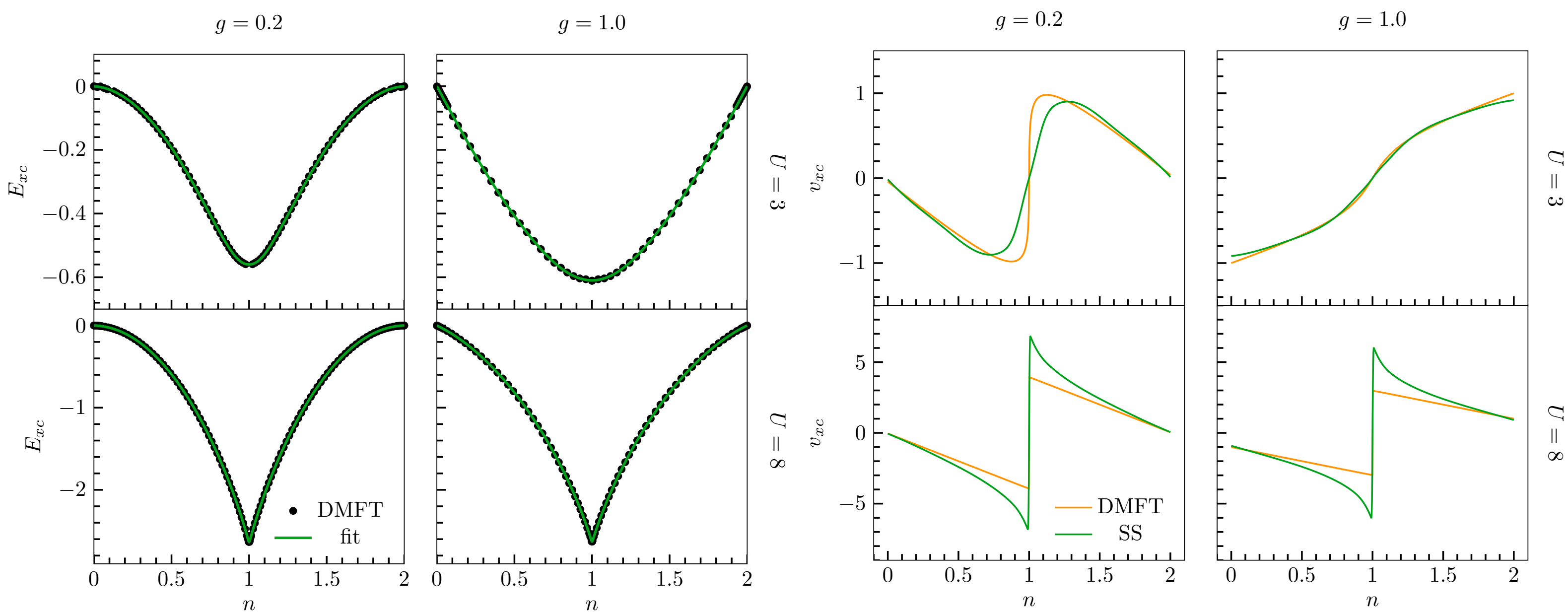
Maps lattice problem to impurity problem

Exact for infinite dimension

$$\lim_{d\to\infty} \Sigma(\mathbf{k},\omega) = \Sigma(\omega)$$

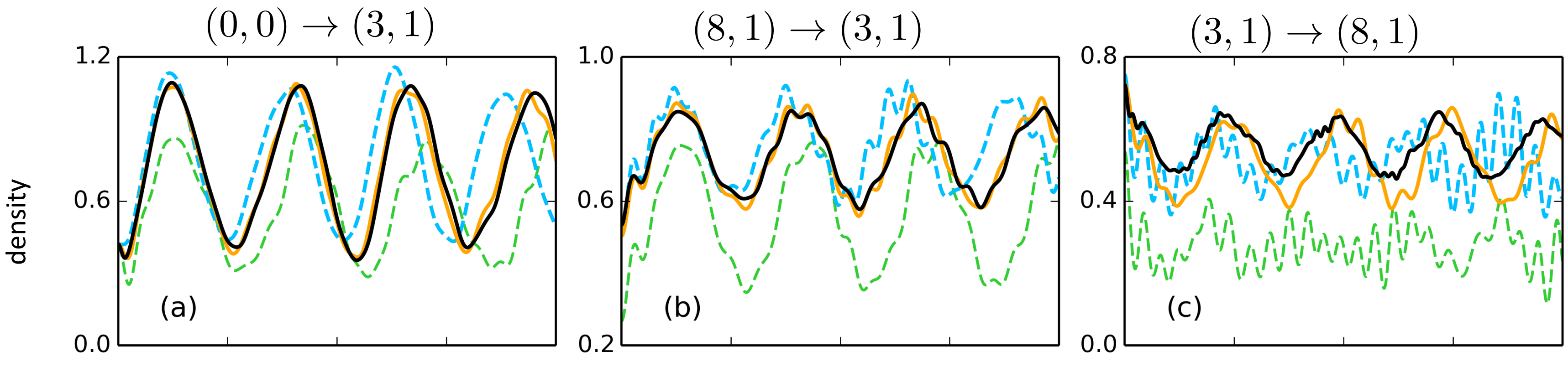
At self-consistency $G_L = G_I$

Non-perturbative, memory but local

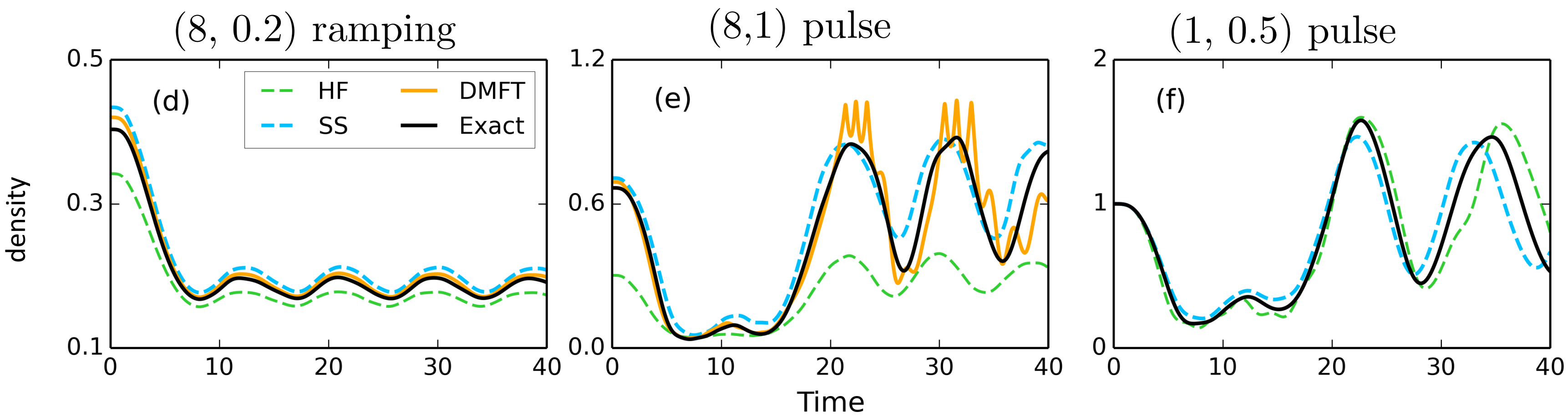


Test Dynamics: TDDFT vs exact **electron density**

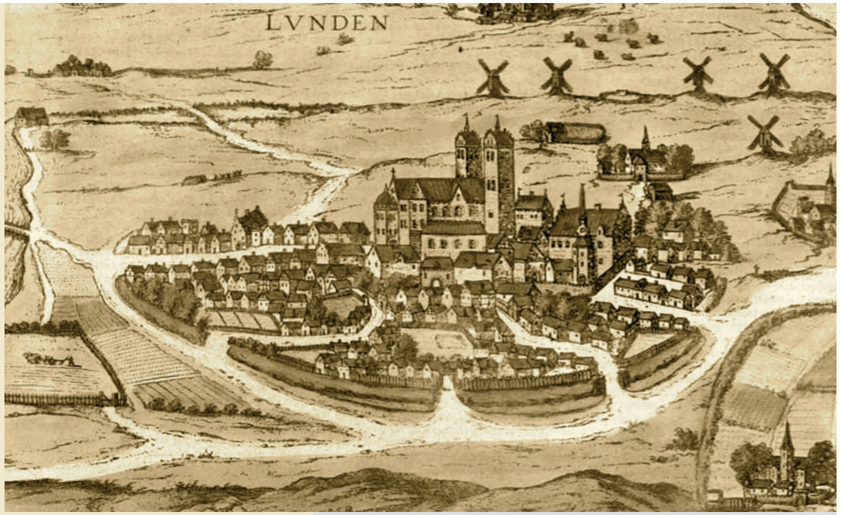
quench (U_i, g_i) --> (U_f, g_f)



external field at impurity site



Summary



GKBA + Ehrenfest dynamics for
Skyrmion dynamics

NEGF for a microscopic picture

- *non-collinear spins:*
- *magnetization dynamics*
- *role of e-e interactions, spin-orbit*

Hurdle

How to deal with localized quantum spins?

Two-component strategy:
can be of some use for localized spins (e.g. skyrmions) ?

In collaboration with: *E. Vinãs Böstrom, P. Helmer, P. Werner*
Thanks to: *G. Stefanucci and E. Perfetto (provided early version of the Cheers code)*