mpsd

Density and kinetic energy density -to- potential mapping on a lattice

Iris Theophilou[1], M. Ruggenthaler [1], F. Bucholz[1], F.G.Eich[1], A. Rubio[1,2]

[1] Max-Planck Institut für Struktur und Dynamik der Materie, Hamburg, Germany

[2] Nano-bio Spectroscopy Group and ETSF, Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, San Sebastian, Spain

New challenges in Reduced Density Matrix Functional Theory: Symmetries, time-evolution and entanglement

RDMFT overview

- ☺ *Explicit expression of kinetic energy, less to approximate*
- ☺ *Fractional occupations make description of static correlation easier*
- ☺*Prediction of TMOs as insulators contrary to DFT*
- ☹ *Pure-N-representability too complicated*
- ☹ *Energy minimization harder than KS DFT*
- ☹ *Absence of auxilary system which can give single particle spectra*

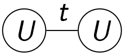
Local RDMFT

- *Local RDMFT* [Lathiotakis et al. *PHYSICAL REVIEW A* 90, 032511 (2014)] *possible way out..*
- *1RDM still basic variable*
- *Natural orbitals taken from a local potential in an OEP way*
- *Natural orbitals approximate*

Minimal Model

mpsd

- Idea of having an intermediate scheme between DFT and RDMFT appealing
- Trying to learn from simple 2-site Hubbard



$$\hat{H} = -t \sum_{\sigma=\uparrow,\downarrow} (\hat{c}^\dagger_{1\sigma}\hat{c}_{2\sigma} + h.c.) + U(\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + \hat{n}_{2\uparrow}\hat{n}_{2\downarrow}) + \cancel{\frac{V}{2}(\hat{n}_1 - \hat{n}_2)}$$

$$\{\hat{c}_{i\sigma}, \hat{c}_{j\sigma'}\} = \delta_{ij}\delta_{\sigma\sigma'}, \quad \hat{n}_{i\uparrow} = \hat{c}^\dagger_{i\uparrow}\hat{c}_{i\uparrow}, \quad \hat{n}_{i\downarrow} = \hat{c}^\dagger_{i\downarrow}\hat{c}_{i\downarrow}$$

Density Matrices in site basis

mpsd

1-RDM in site basis

$$\gamma_{i\sigma,j\sigma'} = tr\{\hat{\rho}\hat{c}_{i\sigma}\hat{c}_{j\sigma'}\}$$

spinless 1-RDM in site basis

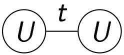
$$\gamma_{i,j} = \sum_{\sigma,\sigma'} tr\{\hat{\rho}\hat{c}_{i\sigma}\hat{c}_{j\sigma'}\}$$

The 2-site Hubbard spinless 1RDM

$$[\gamma_{i,j}] = \begin{bmatrix} n_1 & \gamma(1,2) \\ \gamma(1,2) & n_2 \end{bmatrix}$$

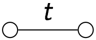
Ground state 1-RDM Hubbard dimer v=0

$$\hat{H} = -t \sum_{\sigma=\uparrow,\downarrow} (\hat{c}^{\dagger}_{1\sigma}\hat{c}_{2\sigma} + h.c.) + U(\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + \hat{n}_{2\uparrow}\hat{n}_{2\downarrow})$$



$$\left[\gamma_{i,j}\right] = \begin{bmatrix} 1 & \frac{4t}{\sqrt{(4t)^2+U^2}} \\ \frac{4t}{\sqrt{(4t)^2+U^2}} & 1 \end{bmatrix}$$

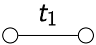
$$\hat{H}^{KS} = -t \sum_{\sigma=\uparrow,\downarrow} (\hat{c}^{\dagger}_{1\sigma}\hat{c}_{2\sigma} + h.c.)$$



$$\left[\gamma^{KS}_{i,j}\right] = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$$

Allowing for different hopping

$$\hat{H}^s = -t_1 \sum_{\sigma=\uparrow,\downarrow} (\hat{c}^\dagger_{1\sigma}\hat{c}_{2\sigma} + h.c.)$$



$$\left[\gamma^s_{i,j}\right] = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$$

- No auxilary non interacting system that can reproduce the GS interacting 1RDM (No surprise!)
- Only with degenerate auxilary natural orbitals we can reproduce interacting γ_{ij} (useless..)
- Control another quantity or consider temperature

Canonical ensemble 1RDM

mpsd

$\gamma(1,2)$ *interacting*

$$\frac{1}{Z}\frac{4t}{\sqrt{(4t)^2+U^2}}e^{-\frac{\beta}{2}U}\left(e^{\frac{\beta\sqrt{(4t)^2+U^2}}{2}}-e^{\frac{-\beta\sqrt{(4t)^2+U^2}}{2}}\right)$$

with $Z = 3 + e^{-\frac{\beta}{2}(U+\sqrt{(4t)^2+U^2})} + e^{-\frac{\beta}{2}(U-\sqrt{(4t)^2+U^2})} + e^{-\beta U}$

$\gamma_s(1,2)$ *non interacting*

$$\frac{1}{Z_s}\left(e^{2\beta t}-e^{-2\beta t}\right)$$

with $Z_s = 4 + e^{-2\beta t} + e^{2\beta t}$

What can we control apart from density?

mpsd

$$\hat{H} = -t \sum_{\sigma=\uparrow,\downarrow} (\hat{c}^{\dagger}_{1\sigma}\hat{c}_{2\sigma} + h.c.) + U(\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + \hat{n}_{2\uparrow}\hat{n}_{2\downarrow})$$

$$\gamma(1,2) = \frac{4t}{\sqrt{4t^2 + U^2}} \quad n_1 = n_2 = 1$$

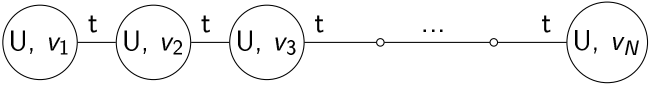
$$\hat{H}^s = -t_1 \sum_{\sigma=\uparrow,\downarrow} (\hat{c}^{\dagger}_{1\sigma}\hat{c}_{2\sigma} + h.c.)$$

$$\gamma(1,2)^s = n_1^s = n_2^s = 1$$

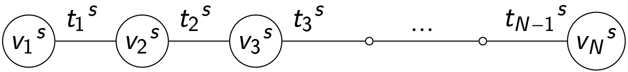
$$Q = t\gamma(1,2) = t_1\gamma(1,2)^s \quad t_1 = \frac{4t^2}{\sqrt{4t^2 + U^2}}$$

Setup

mpsd



$$\hat{H} = -t\sum_{i,\sigma}(\hat{c}^\dagger_{i\sigma}\hat{c}_{i+1\sigma} + h.c.) + U\sum_i \hat{c}^\dagger_{i\uparrow}\hat{c}_{i\uparrow}\hat{c}^\dagger_{i\downarrow}\hat{c}_{i\downarrow} + \sum_{i,\sigma} v_i \hat{c}^\dagger_{i\sigma}\hat{c}_{i\sigma}$$



$$\hat{H}^s = \sum_{i,\sigma} -t_i{}^s(\hat{c}^\dagger_{i\sigma}\hat{c}_{i+1\sigma} + h.c.) + \sum_{i,\sigma} v_i^s \hat{c}^\dagger_{i\sigma}\hat{c}_{i\sigma}$$

$Q_i = \langle\Psi|t\sum_\sigma(\hat{c}^\dagger_{i\sigma}\hat{c}_{i+1\sigma} + h.c.)|\Psi\rangle = \langle\Phi|t_i\sum_\sigma(\hat{c}^\dagger_{i\sigma}\hat{c}_{i+1\sigma} + h.c.)|\Phi\rangle$ and
$n_i = \langle\Psi|\sum_\sigma c^\dagger_{i\sigma}c_{i\sigma}|\Psi\rangle = \langle\Phi|\sum_\sigma c^\dagger_{i\sigma}c_{i\sigma}|\Phi\rangle$

Numerical inversion

$$(t, v_i) \overset{?}{\longleftrightarrow} (Q_i, n_i) \overset{?}{\longleftrightarrow} (t_i^s, v_i^s)$$

- Equations of motion $\langle\Phi|\frac{d^2 n_i}{dt^2}|\Phi\rangle = 0$ $\langle\Phi|\frac{d^2 Q_i}{dt^2}|\Phi\rangle = 0$ connect n_i , Q_i, t_i^s and v_i^s
- Two sites we have ${t_1^s}^2 \Delta n + v_1^s t_1^s \langle\Phi|\hat{c}_1{}^\dagger \hat{c}_2|\Phi\rangle = 0$
- We have done the inversion for 2, 3 and 4 sites

2 site target Δn and Q

$$t_1^{s\,2}(\underbrace{\Delta n}_{\text{target}}) + v_1^s \underbrace{t_1^s\langle\Phi|\hat{c}_1{}^\dagger\hat{c}_2|\Phi\rangle}_{\text{Q target}} = 0$$

Δn and Q from interacting

1. Start from a guess t_1 and v_1
2. $\hat{H} = -t_1\sum_{\sigma=\uparrow,\downarrow}(\hat{c}^\dagger_{1\sigma}\hat{c}_{2\sigma} + h.c.) + v_1(\hat{n}_1 - \hat{n}_2)|\Psi\rangle = \epsilon|\Phi\rangle$

   $$v_1 = -t_1{}^2\overbrace{\Delta n}^{\text{target}} / \overbrace{\langle\Phi|\hat{c}_1{}^\dagger\hat{c}_2|\Phi\rangle}^{\text{updated}}$$
3. Check convergence $|v_1^{old} - v^1| < \epsilon$, if not return to 2
4. $t_1^s = \dfrac{Q}{\langle\Phi|\hat{c}_1{}^\dagger\hat{c}_2|\Phi\rangle}$
5. Rescale $v_1^s = \dfrac{v_1 t_1^s}{t_1}$

Results of inversion Δn and Q

We found an auxilary system $({t_1}^s, {v_1}^s)$ with the same n and Q as interacting

Results of inversion Δn and Q

We found an auxilary system $({t_1}^s, {v_1}^s)$ *with the same* n *and* Q *as interacting*

U=1 t=0.5
$v_1 = 1$

→

$\Delta n = -0.775$
Q=0.435

→

$t_1^s = 0.472$
$v_1^s = 0.397$

and

$t_1^s = -0.472$
$v_1^s = 0.397$

Results of inversion Δn and Q

We found an auxilary system $(t_1{}^s, v_1{}^s)$ with the same n and Q as interacting

U=1 t=0.5
$v_1 = 1$

$\Delta n = -0.775$
Q=0.435

$t_1^s = 0.472$
$v_1^s = 0.397$

$t_1^s = -0.472$
$v_1^s = 0.397$

Is the mapping many to one?

Is the mapping $(t_i^s, v_i^s) \overbrace{\longrightarrow}^{\text{many to one}} (t, v_i)$?

The 3-site lattice single-particle Hamiltonian on site basis:

$$[\mathbf{H}] = \begin{bmatrix} v_1 & t_1 & 0 \\ t_1 & v_2 & t_2 \\ 0 & t_2 & \underbrace{-(v_1 + v_2)}_{\text{from Gauge fixing}} \end{bmatrix}$$

We consider a Unitary transformation $\mathbf{G}$*:*

$$[\mathbf{G}] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Gauge for t_i

mpsd

Transform the initial Hamiltonian $\mathbf{H}' = \mathbf{G}\mathbf{H}\mathbf{G}^{\dagger}$

$$[\mathbf{H}'] = \begin{bmatrix} v_1 & t_1 & 0 \\ t_1 & v_2 & -t_2 \\ 0 & -t_2 & -(v_1 + v_2) \end{bmatrix}$$

Gauge for t_i

Transform the initial Hamiltonian $\mathbf{H}' = \mathbf{G}\mathbf{H}\mathbf{G}^\dagger$

$$[\mathbf{H}'] = \begin{bmatrix} v_1 & t_1 & 0 \\ t_1 & v_2 & -t_2 \\ 0 & -t_2 & -(v_1 + v_2) \end{bmatrix}$$

- *Eigenvalues stay the same, Eigenvectors flip sign from corresponding lattice point and onwards*
- *No physically relevant effect, when hopping changes sign locally*
- *We need to do a Gauge choice for* t_i
- Q_i *does not depend on gauge choice, while 1RDM does!*

Time-dependent Q on a lattice

- Time dependent proved (I. V. Tokatly, PHYSICAL REVIEW B 83, 035127 (2011))
- Many body wavefunction $\Psi(t)[Q, \Psi(0)]$
- Bijective mapping $Q \longleftrightarrow T$
- Time dependent denisty n(t) known from continuity when complex link current Q(t) known

Summary-Outlook

- Which quantities we can control in the minimal setting of 2 site Hubbard with KS type construction?
- Build up a GS theory with basic quantities density and kinetic energy density
- Numerically we have shown existance of auxilary system that reproduces these quantities for few site lattice Hamiltonians
- Gauge choice for hopping

Summary-Outlook

- Time-dependent version on a lattice exits
- In the continuum exact framework for metaGGAs (meaning to position-dependent kinetic energy in GKS)
- In thermal DFT (F G Eich et al 2017 J. Phys.: Condens. Matter 29 063001) "excess energy densities" same in KS and interacting
- In the continuum modelling of materials, macroscopic fluid equations involve kinetic energy density

Thank you for your attention!