Three pieces in RDMFT

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Outline

(1)

An exact functional in RDMFT.

(2)

RDMFT for the Hubbard model.

(3)

Spin spirals within RDMFT.

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Brief recapitulation (Quiz)

One-particle-reduced density matrix (1RDM)

$$\gamma_{\sigma\sigma'}(\boldsymbol{r};\boldsymbol{r}') \equiv \left\langle \hat{c}^{\dagger}_{\sigma'}(\boldsymbol{r}')\,\hat{c}_{\sigma}(\boldsymbol{r})\right\rangle = \sum_{\alpha} n_{\alpha}\phi_{\alpha\sigma}(\boldsymbol{r})\,{\phi^{\star}}_{\alpha\sigma'}(\boldsymbol{r}')\,. \qquad (1)$$

An xc-functional for RDMFT, e. g. Power functional

$$E_{xc}[\gamma] = -\frac{1}{2}\sum_{\alpha\beta}(n_{\alpha}n_{\beta})^{p}\iint \mathrm{d}^3 r_1 \mathrm{d}^3 r_2\, V(\boldsymbol{r}_1,\boldsymbol{r}_2)$$
$$\times\,\mathrm{Tr}[\Phi_{\alpha}(\boldsymbol{r}_1)\,\Phi_{\alpha}(\boldsymbol{r}_2)\,\Phi_{\beta}(\boldsymbol{r}_2)\,\Phi_{\beta}(\boldsymbol{r}_1)]\,. \qquad (2)$$

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$$E_{xc}[\gamma] = -\frac{1}{2}\sum_{\alpha\beta}(n_{\alpha}n_{\beta})^{p} \iint \mathrm{d}^3 r_1 \mathrm{d}^3 r_2\, V(\boldsymbol{r}_1,\boldsymbol{r}_2) \times \mathrm{Tr}[\Phi_{\alpha}(\boldsymbol{r}_1)\,\Phi_{\alpha}(\boldsymbol{r}_2)\,\Phi_{\beta}(\boldsymbol{r}_2)\,\Phi_{\beta}(\boldsymbol{r}_1)]\,. \qquad (2)$$

Part (1)

An exact functional in RDMFT.

The exact functional ... for 2 particles

Singlett wave function

$$\Psi_{\sigma_1\sigma_2}(\boldsymbol{r}_1,\boldsymbol{r}_2) = \psi(\boldsymbol{r}_1,\boldsymbol{r}_2)\,\frac{1}{\sqrt{2}}\{\delta_{\sigma_1\uparrow}\delta_{\sigma_2\downarrow} - \delta_{\sigma_1\downarrow}\delta_{\sigma_2\uparrow}\}\,. \tag{3}$$

Spatial wave function is real, symmetric.

$$\begin{aligned}\psi(\boldsymbol{r}_1,\boldsymbol{r}_2) &= \int \mathrm{d}^3r \underbrace{\sum_\alpha \phi_\alpha(\boldsymbol{r})\,\phi_\alpha(\boldsymbol{r}_1)}_{=\delta(\boldsymbol{r}-\boldsymbol{r}_1)} \psi(\boldsymbol{r},\boldsymbol{r}_2) \\ &= \sum_\alpha c_\alpha(\boldsymbol{r}_2)\,\phi_\alpha(\boldsymbol{r}_1) \\ &= \sum_\alpha c_\alpha\phi_\alpha(\boldsymbol{r}_1)\,\phi_\alpha(\boldsymbol{r}_2)\,. \end{aligned} \tag{4}$$

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By definition

$$\gamma(\boldsymbol{r};\boldsymbol{r}') = \int \mathrm{d}^3 r_2 \psi(\boldsymbol{r},\boldsymbol{r}_2)\,\psi(\boldsymbol{r}',\boldsymbol{r}_2)$$

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$$\times\, \phi_\alpha(\boldsymbol{r}_1)\,\phi_\alpha(\boldsymbol{r}_2)\,\phi_\beta(\boldsymbol{r}_2)\,\phi_\beta(\boldsymbol{r}_1)\,. \quad (6)$$

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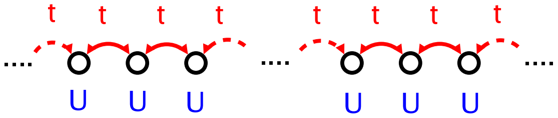
Part (2)

RDMFT for the Hubbard model.

Hubbard model in a nutshell

$$\hat{\mathcal{H}} = -t \sum_{\sigma j} \left\{ \hat{c}^{\dagger}_{j\sigma} \hat{c}_{j+1\sigma} + \hat{c}^{\dagger}_{j+1\sigma} \hat{c}_{j\sigma} \right\} + \frac{1}{2} U \sum_{j\sigma_1\sigma_2} \hat{c}^{\dagger}_{j\sigma_1} \hat{c}^{\dagger}_{j\sigma_2} \hat{c}_{j\sigma_2} \hat{c}_{j\sigma_1} .$$



Why do we investigate the Hubbard model?

- Paradigm for localization induced formation of a gap
- Energy at half filling known from Bethe ansatz solution (BAS)
- Fundamental gap exactly known from BAS

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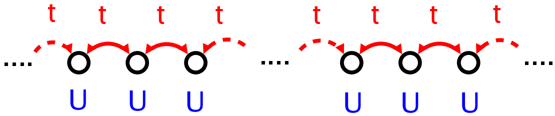

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Particle-hole symmetry in the Hubbard model

Using the anti-commutation relation for fermions we can take the point of view of particles (nomal ordering w.r.t. the vacuum) or the point of view of holes (nomal ordering w.r.t. the *anti*-vacuum).

$$E(n) = E(2-n) + (n-1)\cdot U. \tag{7}$$

Two possibilities

- Either require: $W[\gamma] = W[\mathbb{1}-\gamma] + U(n-1)$
- OR: Define $W[\gamma]$ for particle sector $n \in [0,1]$ and extending it into the hole sector $n \in [1,2]$ using (7)

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A Functional for the Hubbard model derived from the exact functional for the Hubbard dimer

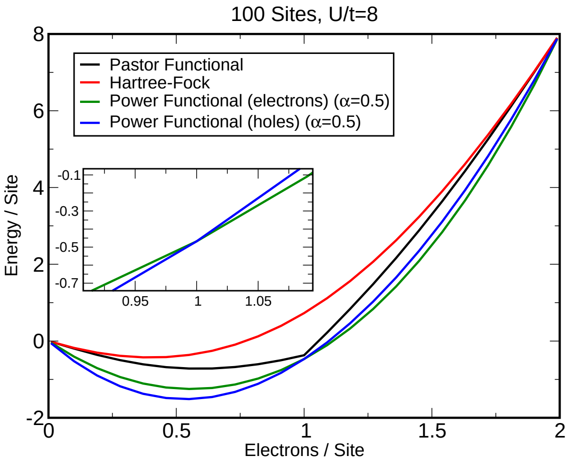
Lopez-Sandoval and Pastor proposed a functional depending *not* on the full 1RDM, but only on the *charge* order (density) n and the 1st *bond* order (kinetic energy density) g
(PRB 66, 155118 (02))

$$W[\gamma] = W(n, g) = U\frac{n^2}{4}\left\{1 - \sqrt{1-(g)^2}\right\},$$

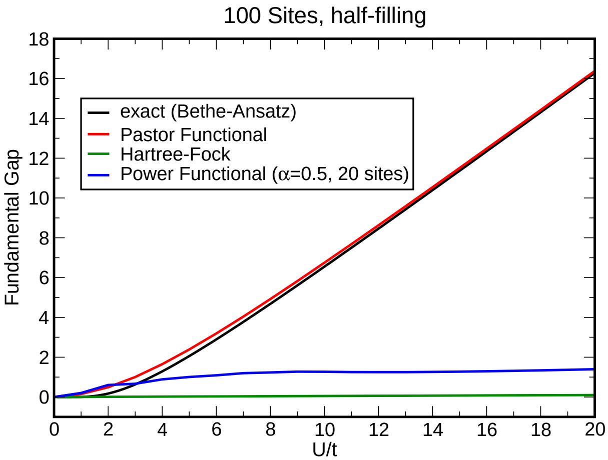
$$n \propto \sum_j \gamma_{jj},$$

$$g \propto \sum_j \left\{\gamma_{j(j+1)} + \gamma_{(j+1)j}\right\}.$$

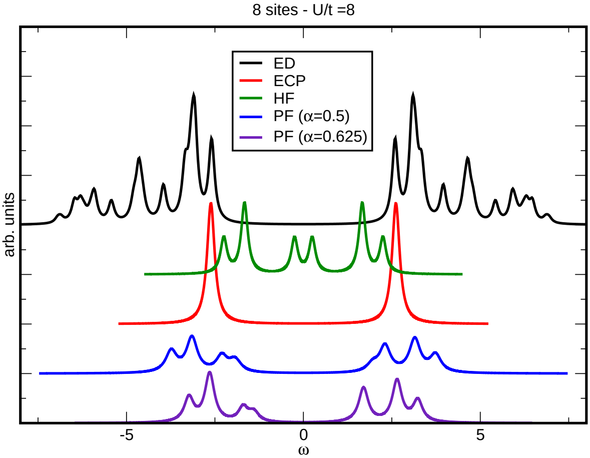
Energy dependent on the filling



Fundamental gap



DOS



Part (3)

Spin spirals within RDMFT.

Overhauser instability

Electron gas has instability w.r.t. the formation of a spin spiral in HF approximation (Overhauser, PR 128 1437 (62))

Overhauser's argument

- Assume potential between spin-up states with $\boldsymbol{k} - \frac{1}{2}\boldsymbol{q}$ and spin-down states with $\boldsymbol{k} + \frac{1}{2}\boldsymbol{q}$ in HF Hamiltonian.
- Demonstrate self-consistency of previous assumption $\rightarrow$ spin spiral orbitals.
- Prove that this spin spiral state has lower energy then the paramagnetic state for q close to $2k_f$.

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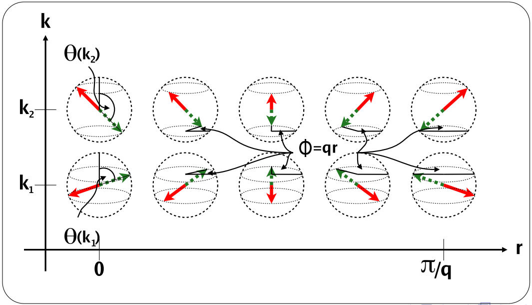
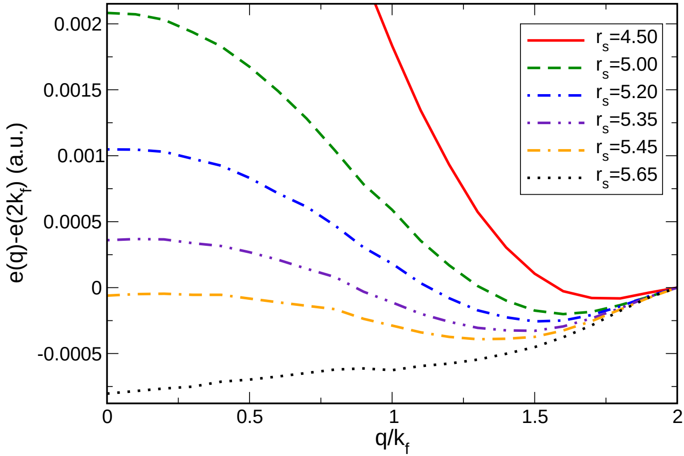
Parametrization of the natural orbitals

$$\phi_{1\boldsymbol{k}}(\boldsymbol{r}) = \frac{1}{(2\pi)^{3/2}} e^{\imath \boldsymbol{k}\cdot\boldsymbol{r}} \begin{pmatrix} \cos\left(\frac{1}{2}\theta(\boldsymbol{k})\right) e^{-\frac{\imath}{2}\boldsymbol{q}\cdot\boldsymbol{r}} \\ \sin\left(\frac{1}{2}\theta(\boldsymbol{k})\right) e^{\frac{\imath}{2}\boldsymbol{q}\cdot\boldsymbol{r}} \end{pmatrix}$$

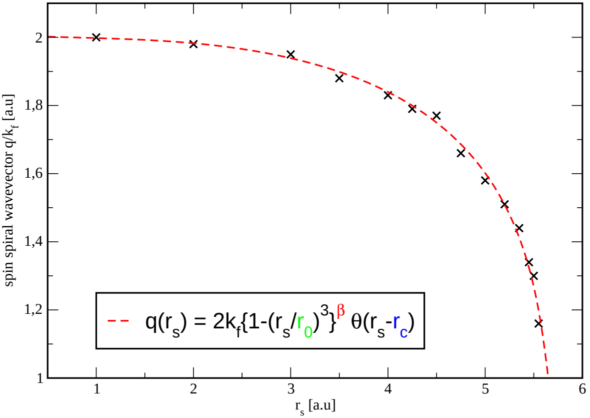
$$\phi_{2\boldsymbol{k}}(\boldsymbol{r}) = \frac{1}{(2\pi)^{3/2}} e^{\imath \boldsymbol{k}\cdot\boldsymbol{r}} \begin{pmatrix} -\sin\left(\frac{1}{2}\theta(\boldsymbol{k})\right) e^{-\frac{\imath}{2}\boldsymbol{q}\cdot\boldsymbol{r}} \\ \cos\left(\frac{1}{2}\theta(\boldsymbol{k})\right) e^{\frac{\imath}{2}\boldsymbol{q}\cdot\boldsymbol{r}} \end{pmatrix}$$



Dependence of the ground-state energy on the spin spiral wave vector



Dependence of the optimal spin spiral wave vector on the density

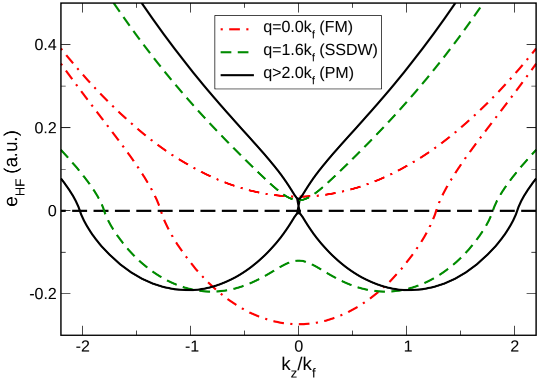


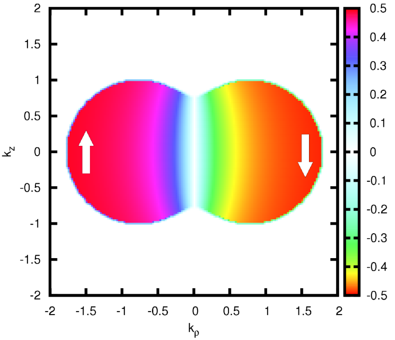
$\beta \approx 0.2$

$r_0 \approx 5.7$

$r_c \approx 5.56$

HF dispersion, Fermi surface and angular function $r_s = 5$





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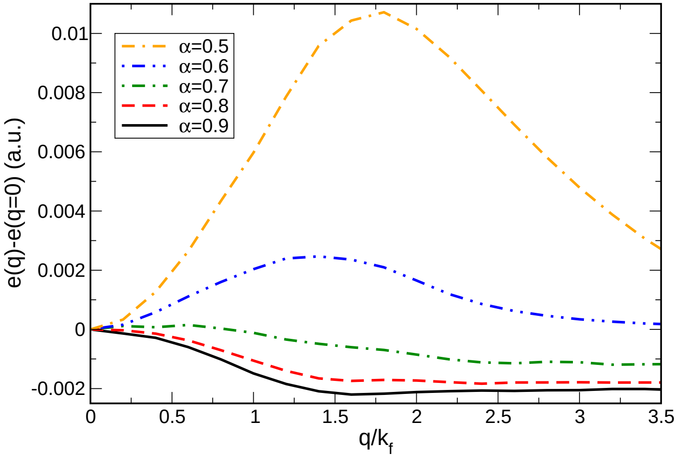

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