One-Matrix functional theory

$$\gamma(r,r') = N\int dr_2 \ldots dr_N \Psi_0^*(r,r_2,\ldots r_N)\Psi_0(r',r_2,\ldots r_N)$$

$$E_v[\gamma] = T[\gamma] + \int drdr' v(r,r')\gamma(r',r) + E_{int}[\gamma]$$

Is there a Kohn-Sham system?

$$\gamma(r,r') = \sum_j^{occ} \phi_j(r)\phi_j^*(r') \qquad \gamma(r,r') = \sum_j f_j\phi_j(r)\phi_j^*(r')$$

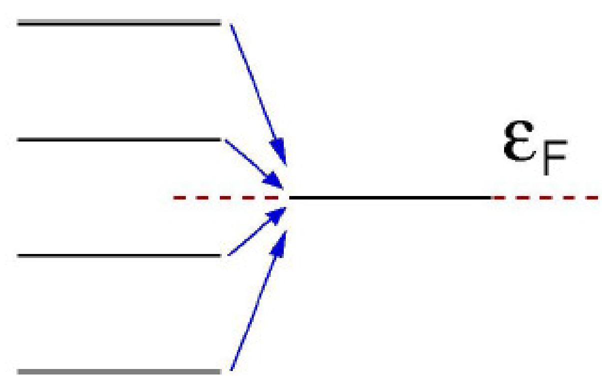
$$\hat{h} = \frac{\delta E_v}{\delta\gamma} = -\frac{1}{2m}\nabla^2 + \int dr'\; v_s(r,r')$$

$$v_s(r,r') = v(r,r') + \frac{E_{int}}{\delta\gamma(r',r)}$$

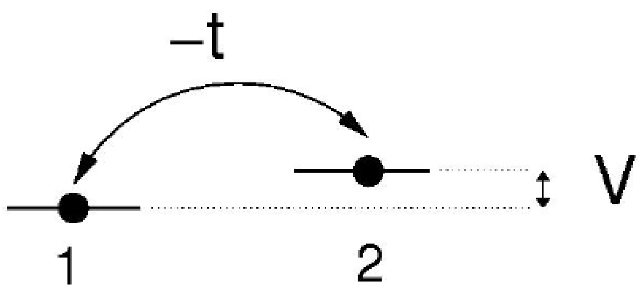
Total degeneracy

$$\frac{\partial E_v}{\partial f_j} = \epsilon_F$$

$$\Rightarrow \hat{h} \to \epsilon_F \hat{1}$$

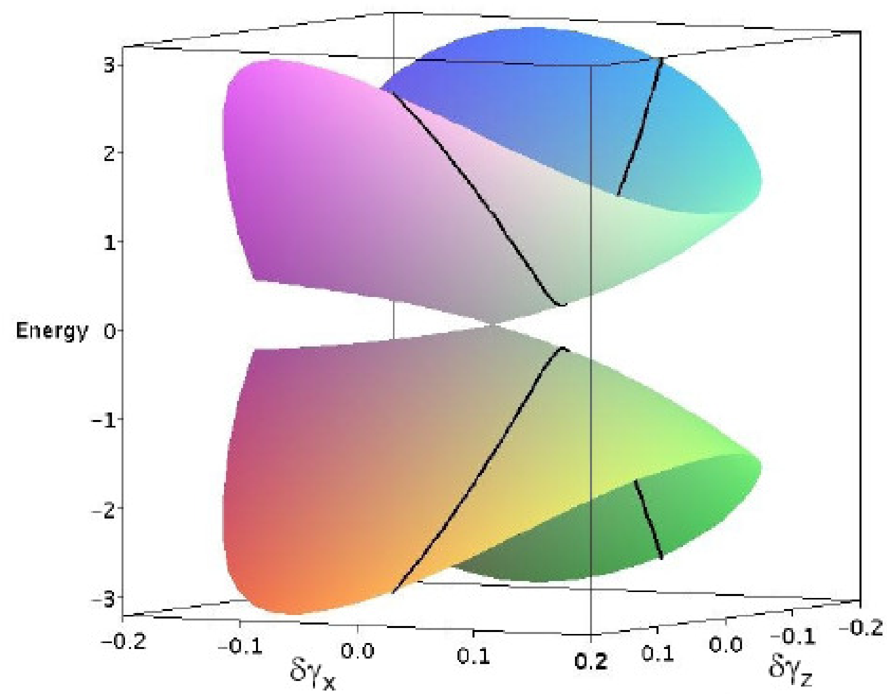


Example: 2-site Hubbard model



$$E_s[\gamma] = Tr(\hat{h}\hat{\gamma}) = \sum_j f_j \epsilon_j$$

$$\gamma_{j\sigma k\nu} = \left\langle \Psi_0 \left| c^\dagger_{j\sigma} c_{k\nu} \right| \Psi_0 \right\rangle$$



$$A = \frac{1}{2}(f_a - f_b)$$

$$A - A_0 = 0.03$$

Equations of motion

$$i\partial_t \gamma(x_1, x_1'; t) = (\hat{h}_0(x_1, t) - \hat{h}_0(x_1', t))\gamma(x_1, x_1'; t) + $$
$$+ 2\int dx_2 (v_c(x_1, x_2) - v_c(x_1', x_2))\Gamma(x_1, x_2, x_1', x_2; t)$$

$$i\partial_t |\phi_k\rangle = (\hat{t} + \hat{v}_{eff})|\phi_k\rangle$$

$$i\partial_t f_k = \langle \phi_k | \hat{w} | \phi_k \rangle \qquad w(x, x') = 2\int dy (v_c(x, y) - v_c(x', y))\Gamma(x, y, x', y; t)$$

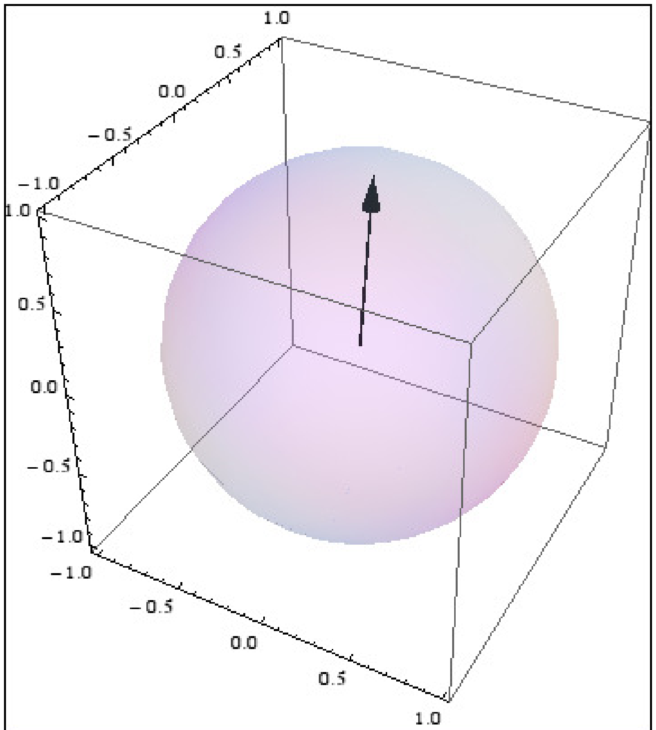
Müller functional

$$V_{ee} = \frac{1}{2}\sum \iint dr dr' \left[f_j f_k \frac{\phi_j^*(r)\phi_k^*(r')\phi_j(r)\phi_k(r')}{|r - r'|} - \sqrt{f_j f_k} \frac{\phi_j^*(r)\phi_k^*(r')\phi_k(r)\phi_j(r')}{|r - r'|} \right]$$

for $\hat{\Gamma}_{ijkl} = F_{ijij}\delta_{ik}\delta_{jl} + G_{ijji}\delta_{il}\delta_{jk}$ $\qquad i\partial_t f_k = \langle \phi_k | \hat{w} | \phi_k \rangle = 0$

Linear time dependence $V_3 = \alpha t$

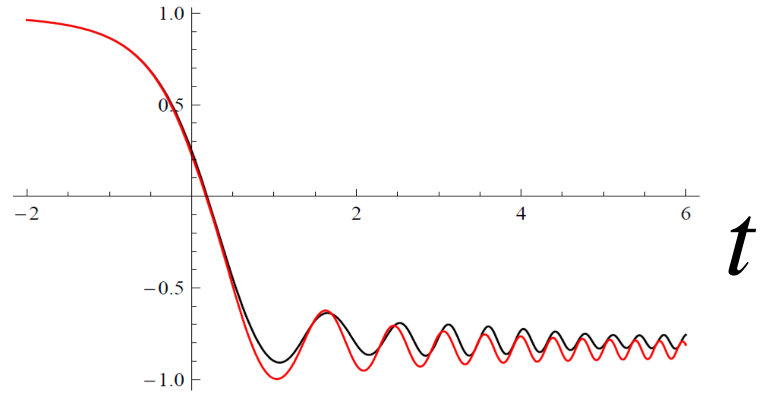
$$\dot{\vec{\gamma}} = \vec{V} \times \vec{\gamma} + \vec{W} \qquad \vec{V} = (-2b, 0, V_3(t)) \qquad \vec{W}(t) = W(\varphi(t), \theta(t), |\gamma(t)|)$$



Animation a2 U2

$$\alpha = 2, U = 2$$

$$\gamma_3 = (n_1 - n_2)/2$$



$$|\gamma| = (f_a - f_b)/2$$