Illustration of the Geometric Principle in TDDFT with a 1D Soft-Coulomb Model

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1D Soft-Coulomb Model with 2 electrons in a spin singlet state

Interacting system

$\Psi^S(t) = \Psi^S(t, x_1, x_2)$ symmetric

$$\begin{cases} i\partial_t \Psi^S(t) = \widehat{H}^S(t)\Psi^S(t) \\ \Psi^S(0) = \Psi_0 \end{cases}$$

$\widehat{H}^S(t) := \sum_{i=1}^2 \widehat{h}(t, x_i) + \underbrace{\frac{1}{\sqrt{(x_1-x_2)^2+1}}}_{\text{Soft-Coulomb}}$

$\Rightarrow$ Gives ρ^S

Kohn–Sham system

One spatial orbital $\varphi(t) = \varphi(t, x)$

$$\begin{cases} i\partial_t \varphi(t) = (\widehat{h}(t) + \widehat{\mathbf{F}}(\mathbf{t}))\varphi(t) \\ \varphi(0) = \varphi_0 \end{cases}$$

$\widehat{h}(t) = -\frac{1}{2}\partial_x^2 + V_{\text{ext}}(t, x)$

$\Rightarrow$ Gives $\rho_\varphi = 2|\varphi|^2$

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Several choices for $\widehat{\mathbf{F}}(\mathbf{t})$ to enforce $\rho^S = \rho_\varphi$:

1. **Variational Principle** : $\widehat{\mathbf{F}}(\mathbf{t}) = \mathbf{V}(\mathbf{t}, \mathbf{x})$
2. **Geometric Principle** : $\widehat{\mathbf{F}}(\mathbf{t}) = \mathbf{i}\mathbf{W}(\mathbf{t}, \mathbf{x})$
3. **We can mix both** : $\widehat{\mathbf{F}}(\mathbf{t}) = \mathbf{V}(\mathbf{t}, \mathbf{x}) + \mathbf{i}\mathbf{W}(\mathbf{t}, \mathbf{x})$

(for e.g. W^{corr} can correct $V_{\text{adia}}^{\text{approx}}$)

Hydrodynamic picture

If $\rho_\varphi = \rho^S$, one can write **the polar form**

$$\boxed{\varphi(t,x) = \sqrt{\frac{\rho^S(t,x)}{2}}\, e^{i\theta(t,x)}}$$

The non–interacting current is $j_\varphi = j_\theta := \rho^S \partial_x \theta$.

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Then the triplet $(\theta, \mathbf{V}, \mathbf{W})$ solves the hydrodynamic equations

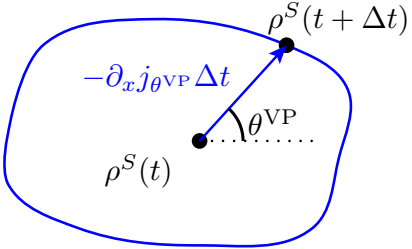
$$\boxed{\begin{cases} \mathbf{W} = \dfrac{\partial_t \rho^S + \partial_x(\rho^S \partial_x \theta)}{2\rho^S}, \\ \mathbf{V} = -\partial_t \theta - \dfrac{|\partial_x \theta|^2}{2} + \dfrac{\partial_x^2 \sqrt{\rho^S}}{2\sqrt{\rho^S}} - V_{\text{ext}}. \end{cases}}$$

$V^{\text{eaKS}} := \dfrac{\partial_x^2 \sqrt{\rho^S}}{2\sqrt{\rho^S}} - V_{\text{ext}}$ is the **exact adiabatic Kohn-Sham potential** giving ρ^S.

Hydrodynamic picture : VP vs GP

Variational Principle : set W = 0
$\rightarrow$ the pair $(\theta^{\mathrm{VP}}, \mathbf{V}^{\mathrm{eKS}})$ solves

$$\begin{cases} \mathbf{0} = \dfrac{\partial_t \rho^S + \partial_x(\rho^S \partial_x \theta^{\mathrm{VP}})}{2\rho^S}, \\ \mathbf{V}^{\mathrm{eKS}} = -\partial_t \theta^{\mathrm{VP}} - \dfrac{|\partial_x \theta^{\mathrm{VP}}|^2}{2} + V^{\mathrm{eaKS}}. \end{cases}$$



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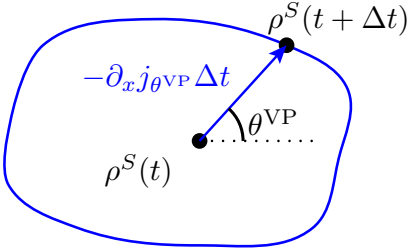
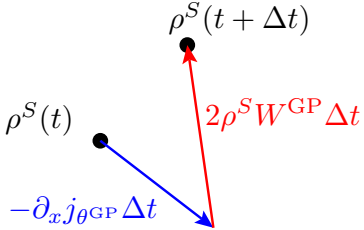


Geometric Principle : set V = 0
$\rightarrow$ the pair $(\theta^{\mathrm{GP}}, \mathbf{W}^{\mathrm{GP}})$ solves

$$\begin{cases} \mathbf{W}^{\mathrm{GP}} = \dfrac{\partial_t \rho^S + \partial_x(\rho^S \partial_x \theta^{\mathrm{GP}})}{2\rho^S}, \\ \mathbf{0} = -\partial_t \theta^{\mathrm{GP}} - \dfrac{|\partial_x \theta^{\mathrm{GP}}|^2}{2} + V^{\mathrm{eaKS}}. \end{cases}$$

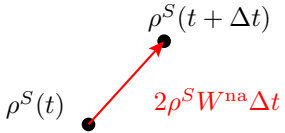


GP as a correction to exact adiabatic

A third natural choice : set $\theta = 0$! $\rightarrow$ No equation to solve !

The pair $(\mathbf{V}^{\mathrm{eaKS}}, \mathbf{W}^{\mathrm{na}})$ is directly given by

$$\begin{cases} \mathbf{W}^{\mathrm{na}} = \dfrac{\partial_t \rho^S}{2\rho^S}, \\ \mathbf{V}^{\mathrm{eaKS}} = \dfrac{\partial_x^2 \sqrt{\rho^S}}{2\sqrt{\rho^S}} - V_{\mathrm{ext}}. \end{cases}$$



$\mathbf{W}^{\mathrm{na}}$ **is the non-adiabatic correction to the exact adiabatic potential** $\mathbf{V}^{\mathrm{eaKS}}$.

What does W^{na} look like ?

We want to compare $\mathbf{V}^{\mathrm{na}} := \mathbf{V}^{\mathrm{eKS}} - \mathbf{V}^{\mathrm{eaKS}}$ and $\mathbf{W}^{\mathrm{na}}$.

The shape of $\mathbf{V}^{\mathrm{na}}$ has already been studied to understand what is missing in current approximations (for e.g. steps).

See the works of

- P. Elliott et al. "Universal Dynamical Steps in the Exact Time-Dependent Exchange-Correlation Potential". In: *Phys. Rev. Lett.* 109.26 (Dec. 2012), p. 266404
- N. Helbig et al. "Density functional theory beyond the linear regime: Validating an adiabatic local density approximation". In: *Phys. Rev. A* 83.3 (Mar. 2011), p. 032503
- N. Helbig et al. "Time-dependent density-functional and reduced density-matrix methods for few electrons: Exact versus adiabatic approximations". In: *Chem. Phys.* 391.1 (Nov. 2011), pp. 1–10
- J. I. Fuks et al. "Nonlinear phenomena in time-dependent density-functional theory: What Rabi oscillations can teach us". In: *Phys. Rev. B* 84.7 (Aug. 2011), p. 075107

1D Helium Atom

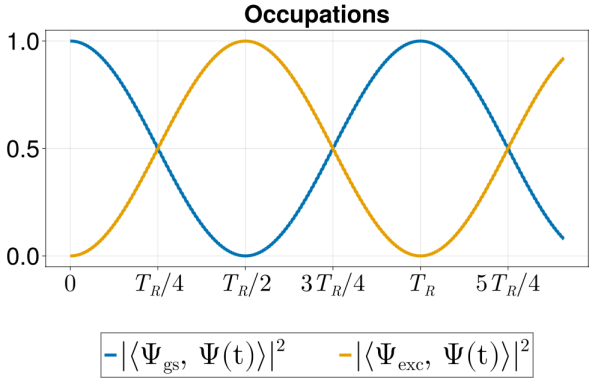
Helium atom with electric field :

$$V_{\text{ext}}(t,x) = -\frac{2}{\sqrt{x^2+1}} + Ex\sin(\omega t)$$

ω chosen to induce **Rabi Oscillations**

$$\Psi_{\text{gs}} \xrightarrow{T_R/2} \Psi_{\text{exc}} \xrightarrow{T_R/2} \Psi_{\text{gs}} \xrightarrow{T_R/2} \cdots$$

with Ψ_{gs} = ground state
Ψ_{exc} = first excited state
T_R = Rabi period.

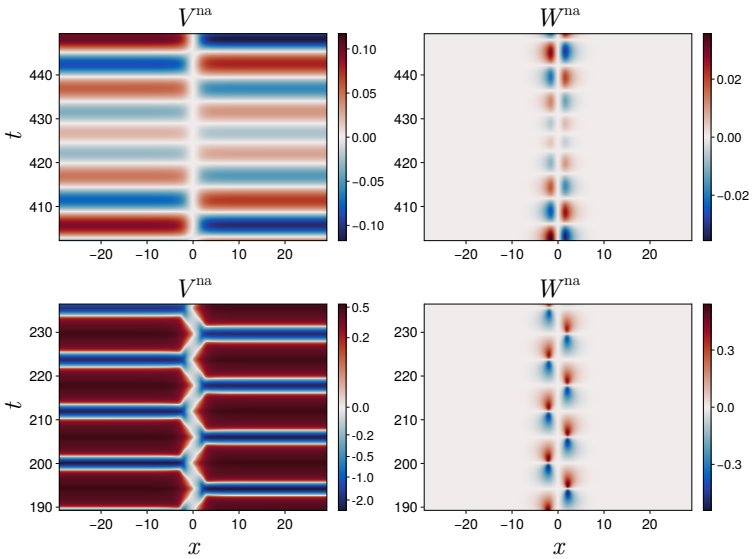


We simulate the interacting system to get the interacting density ρ^S.

Rabi Oscillations in 1D Helium

around $T_R/2$

around $T_R/4$



Thank you for your attention !