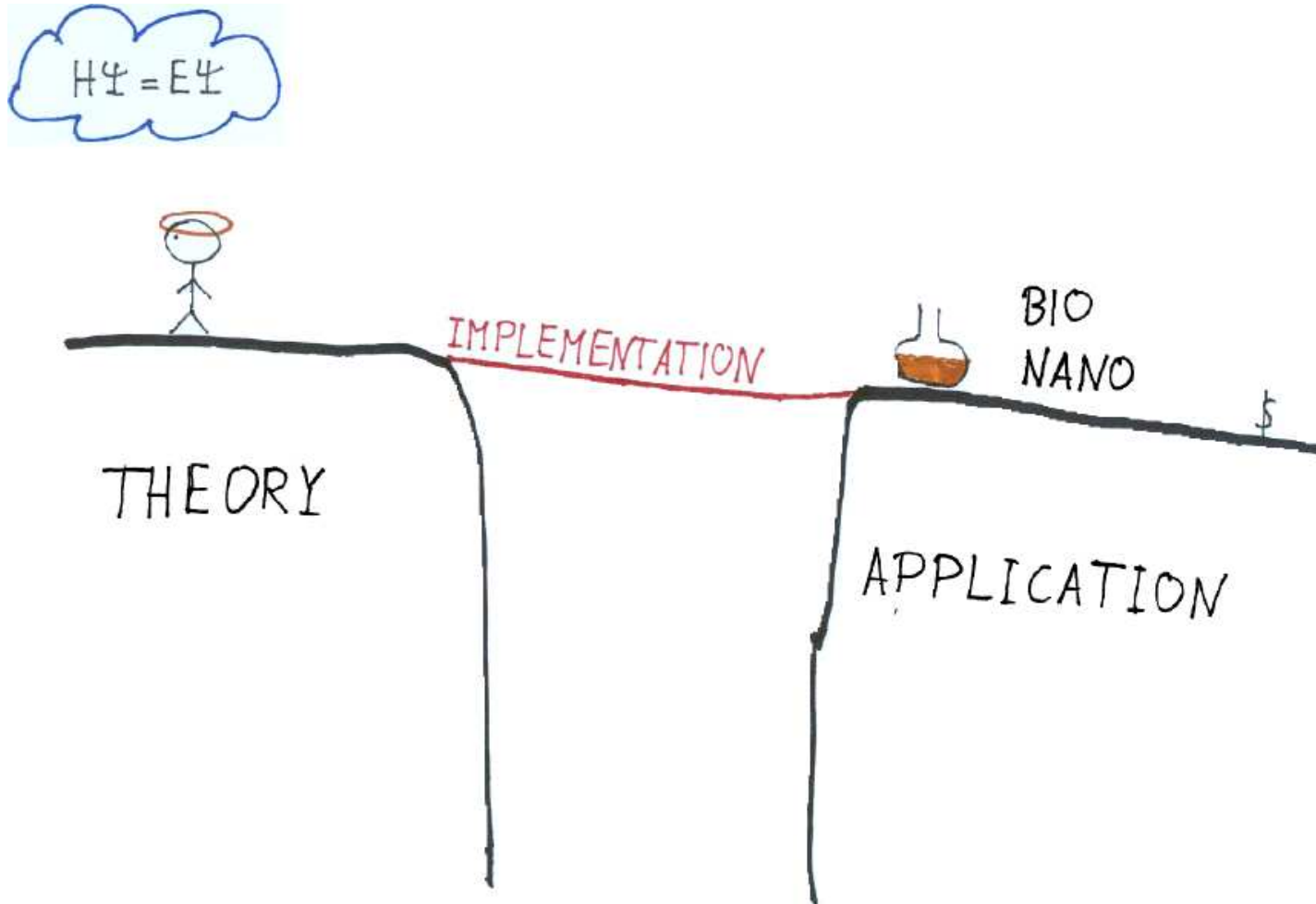


# **Efficient computation of molecular response and excited state properties**

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## Bridging the gap



# Working equations

# Density-matrix based response theory I

- Basic variable: The **non-interacting** TDKS density matrix

$$\gamma(t, x, x') = \sum_{j=1}^N \varphi_j(t, x) \varphi_j^*(t, x')$$

- **Physical** time-dependent density and current density accessible (cf. previous talks),

$$\rho(t, x) = \gamma(t, x, x),$$

$$\mathbf{j}(t, x) = 1/2 [\boldsymbol{\pi}(t, x) + \boldsymbol{\pi}^*(t, x')] \gamma(t, x, x') \Big|_{x'=x}$$

- Equations of motion:

$$i \frac{\partial}{\partial t} \gamma(t) = [H_{\text{KS}}(t), \gamma(t)]$$

$$\gamma(t) = \gamma^2(t)$$

## Density-matrix based response theory II

- Periodic perturbation with coupling constant  $\lambda$ ,

$$H_{\text{KS}\lambda}(t) = \frac{1}{2}\pi^2(t) + v_{\text{ext}}^{(0)}(x) + \int dx' \frac{\rho_\lambda(t, x')}{|\mathbf{r} - \mathbf{r}'|} + v^{\text{xc}}[\rho_\lambda](t, x) - c_x v^{\text{x, HF}}[\gamma_\lambda](t) \\ + \lambda(\hat{v}^{(1)}(\omega, x)e^{i\omega t} + \hat{v}^{(1)}(-\omega, x)e^{-i\omega t})$$

- Response properties from order-by-order solution of the equations of motion for  $\gamma_\lambda(t)$
- Advantages:
  - Unitary invariant version of TDKS scheme
  - Response from straightforward differentiation
  - No response functions, no orbital derivatives, efficient implementation
  - Straightforward matrix equivalent
  - Efficient ground-state density matrix techniques transferable

F. F., *J. Chem. Phys.* **114** (2001), 5982.

## Frequency dependence

- Notation:

$$\gamma^{(n)}(t) = \frac{1}{n!} \left. \frac{\partial}{\partial \lambda} \gamma_\lambda(t) \right|_{\lambda=0}$$

- Since the external perturbing potential is periodic with frequency  $\omega$ , the  $n$ -th order response has characteristic periodicity:

$$\gamma^{(0)}(t) = \gamma^{(0)}$$

$$\gamma^{(1)}(t) = \hat{\gamma}^{(1)}(\omega) e^{i\omega t} + \hat{\gamma}^{(1)}(-\omega) e^{-i\omega t}$$

$$\gamma^{(2)}(t) = \hat{\gamma}^{(2)}(\omega, \omega) e^{2i\omega t} + \hat{\gamma}^{(2)}(\omega, -\omega) + \hat{\gamma}^{(2)}(-\omega, \omega) + \hat{\gamma}^{(2)}(-\omega, -\omega) e^{-2i\omega t}$$

⋮

## Zeroth order: Static KS

- Zeroth order idempotency constraint,

$$\gamma^{(0)} = \gamma^{(0)}\gamma^{(0)},$$

equivalent to spectral representation

$$\gamma^{(0)}(x, x') = \sum_{i=1}^N \varphi_i(x)\varphi_i(x')$$

- Zeroth order EOM,

$$0 = [H_{\text{KS}}^{(0)}, \gamma^{(0)}],$$

equivalent to static (hybrid) KS equations,

$$H_{\text{KS}}^{(0)}\varphi_i(x) = \epsilon_i\varphi_i(x)$$

# First order: Linear response I

- First order idempotency constraint:

$$\hat{\gamma}^{(1)} = \gamma^{(0)} \hat{\gamma}^{(1)} + \hat{\gamma}^{(1)} \gamma^{(0)}$$

- Static KS orbital basis:

$$\hat{\gamma}^{(1)}(x, x') = \sum_{ia} (X_{ia} \varphi_a(x) \varphi_i(x') + Y_{ia} \varphi_i(x) \varphi_a(x'))$$

- $\hat{\gamma}^{(1)} \in L = L_{\text{virt}} \otimes L_{\text{occ}} \oplus L_{\text{occ}} \otimes L_{\text{virt}}$ :

$$\gamma^{(1)} = \begin{pmatrix} X \\ Y \end{pmatrix} = |X, Y\rangle$$

- Since  $\gamma^{(1)}(t) = \gamma^{(1)\dagger}(t)$  we have

$$X(\omega) = Y(-\omega)$$

$$Y(\omega) = X(-\omega)$$



## First order: Linear response II

- First order EOM:

$$\omega \hat{\gamma}^{(1)} = [H_{\text{KS}}^{(0)}, \hat{\gamma}^{(1)}] + [\hat{H}_{\text{KS}}^{(1)}, \gamma^{(0)}]$$

- Functional chain rule:

$$\begin{aligned} \hat{H}_{\text{KS}}^{(1)}(\omega) = & \int dx' \left( \frac{1}{|\mathbf{r} - \mathbf{r}'|} + f^{\text{xc}}(\omega, x, x') \right) \hat{\rho}^{(1)}(\omega, x') - c_x v^{\text{x, HF}}[\hat{\gamma}^{(1)}](\omega) \\ & + \hat{v}^{(1)}(\omega, x) \end{aligned}$$

- Adiabatic approximation:

$$f^{\text{xc}}(\omega, x, x') = f^{\text{xc}}(0, x, x') = \frac{\delta^2 E^{\text{xc}}}{\delta \rho(x) \delta \rho(x')}$$

## First order: Linear response III

- EOM in static KS orbital basis:

$$(\Lambda - \omega\Delta)|X, Y\rangle = -|P, Q\rangle$$

- Super-operators:

$$\Lambda = \begin{pmatrix} A & B \\ B & A \end{pmatrix}, \quad \Delta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

- Orbital rotation Hessians:

$$(A + B)_{iajb} = (\epsilon_a - \epsilon_i)\delta_{ij}\delta_{ab} + 2\langle ab|ij\rangle + 2f_{iajb}^{\text{xc}} - c_x[\langle ab|ji\rangle + \langle aj|bi\rangle]$$

$$(A - B)_{iajb} = (\epsilon_a - \epsilon_i)\delta_{ij}\delta_{ab} + c_x[\langle ab|ji\rangle - \langle aj|bi\rangle]$$

- External perturbation:

$$(P + Q)_{ia} = 2\langle i|\hat{v}^{(1)}(\omega)|a\rangle, \quad (P - Q)_{ia} = 0$$

## First order: Linear response IV

- Example: Polarizability  $\alpha_{ij}(\omega)$

$$|P, Q\rangle = |\mu_j\rangle$$

$$\alpha_{ij}(\omega) = \langle \mu_i | X, Y \rangle = \langle \mu_i | (\Lambda - \omega \Delta)^{-1} | \mu_j \rangle$$

- Hylleraas variational principle: Find stationary point of

$$F[X, Y] = \langle X, Y | \Lambda - \omega \Delta | X, Y \rangle + \langle X, Y | P, Q \rangle + \langle P, Q | X, Y \rangle$$

- First variation of  $F$ :

$$\frac{\delta F[X, Y]}{\delta \langle X, Y |} = (\Lambda - \omega \Delta) | X, Y \rangle + | P, Q \rangle = 0$$

## Higher order

- $n$ -th order idempotency constraint: occ-occ and virt-virt parts of  $\hat{\gamma}^{(n)}$  are products of lower-order quantities
- $n$ -th order EOM: occ-virt and virt-occ part  $|X^{(n)}, Y^{(n)}\rangle$  satisfies

$$(\Lambda - \omega\Delta)|X^{(n)}, Y^{(n)}\rangle = -|P^{(n-1)}, Q^{(n-1)}\rangle,$$

where  $|P^{(n-1)}, Q^{(n-1)}\rangle$  contains lower-order quantities

- $\hat{\gamma}^{(n)}$  determines (quasi-)energy to order  $2n + 1$  (Wigner's rule)

# Excited states I

- First order response of the TDKS density matrix

$$|X, Y\rangle = -(\Lambda - \Omega\Delta)^{-1}|P, Q\rangle$$

diverges if  $\omega \rightarrow \Omega_n$ .

- Determine poles and residues of  $(\Lambda - \Omega\Delta)^{-1}$ :

$$(\Lambda - \Omega_n\Delta)|X_n, Y_n\rangle = 0, \quad \langle X_n, Y_n|\Delta|X_n, Y_n\rangle = 1$$

- $\Omega_n$  **interacting** excitation energies
- $|X_n, Y_n\rangle$  yields **interacting** transition (current) densities or “collective density modes”
- Examples: Oscillator and rotatory strength

$$f_{0n} = \frac{2}{3}\Omega_n |\langle \boldsymbol{\mu} | X_n, Y_n \rangle|^2$$

$$R_{0n} = \text{Im} \langle \boldsymbol{\mu} | X_n, Y_n \rangle \cdot \langle X_n, Y_n | \mathbf{m} \rangle$$

## Excited states II

- Hylleraas variational principle: Find stationary point of

$$G[X, Y, \Omega] = \langle X, Y | \Lambda | X, Y \rangle - \Omega (\langle X, Y | \Delta | X, Y \rangle - 1)$$

- First variation of  $G$ :

$$\frac{\delta G[X, Y, \Omega]}{\delta \langle X, Y |} = (\Lambda - \Omega \Delta) | X, Y \rangle = 0$$
$$\frac{\partial G[X, Y, \Omega]}{\partial \Omega} = \langle X, Y | \Delta | X, Y \rangle - 1$$

- Sum rules from spectral representation

$$(\Lambda - z\Delta)^{-1} = \sum_n \left( \frac{1}{\Omega_n - z} |X_n, Y_n\rangle \langle X_n, Y_n| + \frac{1}{\Omega_n + z} |Y_n, X_n\rangle \langle Y_n, X_n| \right)$$

## Summary

- TDDFT is based on a mapping of the interacting problem on the non-interacting TDKS system (cf. previous talks)
- Response properties of the interacting system can be extracted from the TDKS response
- The central equation of TDKS response theory is (TDKS response equation)

$$(\Lambda - \omega\Delta)|X, Y\rangle = -|P, Q\rangle$$

- Excitation energies and transition moments are accessible from the poles of the TDKS density matrix response
- The central equation of TDKS excited state theory is (TDKS eigenvalue problem, “Casida’s equations”)

$$(\Lambda - \Omega\Delta)|X, Y\rangle = 0, \quad \langle X, Y|\Delta|X, Y\rangle = 1$$

# Implementation



# Discretization

- Generate a **finite** number of MOs by the LCAO-MO expansion,

$$\phi_{p\sigma}(\mathbf{r}) = \sum_{\mu} C_{\mu p\sigma} \chi_{\mu}(\mathbf{r})$$

- TDKS response/eigenvalue problem becomes **finite dimensional** linear equation system/eigenvalue problem  $\rightarrow$  matrix algebra
- Basis set error, can be controlled by extrapolation
- Contracted Cartesian Gaussians, the better choice for molecules:

$$\chi_{\mu}(\mathbf{r}) = \sum_p c_p x^i y^j z^k e^{-\zeta_p (\mathbf{r} - \mathbf{R}_{\mu})^2}$$

- Gaussian product theorem  $\rightarrow$  multi-center integrals
- Hermite recursion: Higher  $l$  quantum numbers from derivatives with respect to  $\mathbf{R}_{\mu}$

## Solution by elimination techniques

$$(A + B)_{ia\sigma jb\sigma'} = (\epsilon_{a\sigma} - \epsilon_{i\sigma})\delta_{ij}\delta_{ab}\delta_{\sigma\sigma'} + 2(ia\sigma|jb\sigma') + 2f_{ia\sigma jb\sigma'}^{\text{xc}} - c_x\delta_{\sigma\sigma'}[(ja\sigma|ib\sigma) + (ab\sigma|ij\sigma)]$$

$$(A - B)_{ia\sigma jb\sigma'} = (\epsilon_{a\sigma} - \epsilon_{i\sigma})\delta_{ij}\delta_{ab}\delta_{\sigma\sigma'} + c_x\delta_{\sigma\sigma'}[(ja\sigma|ib\sigma) - (ab\sigma|ij\sigma)]$$

The dimension of  $L$  scales as  $N_{\text{occ}} \cdot N_{\text{virt}}$ !

Naive approach:

- Calculate all integrals and store them  $\rightarrow$  CPU  $\sim N^5$ , I/O  $\sim N^4$
- Use elimination techniques to solve the linear equation system / eigenvalue problem  $\rightarrow$  CPU  $\sim N^6$

Prohibitive for more than 10 atoms

The end of TDDFT (in chemistry)!

## Iterative Methods

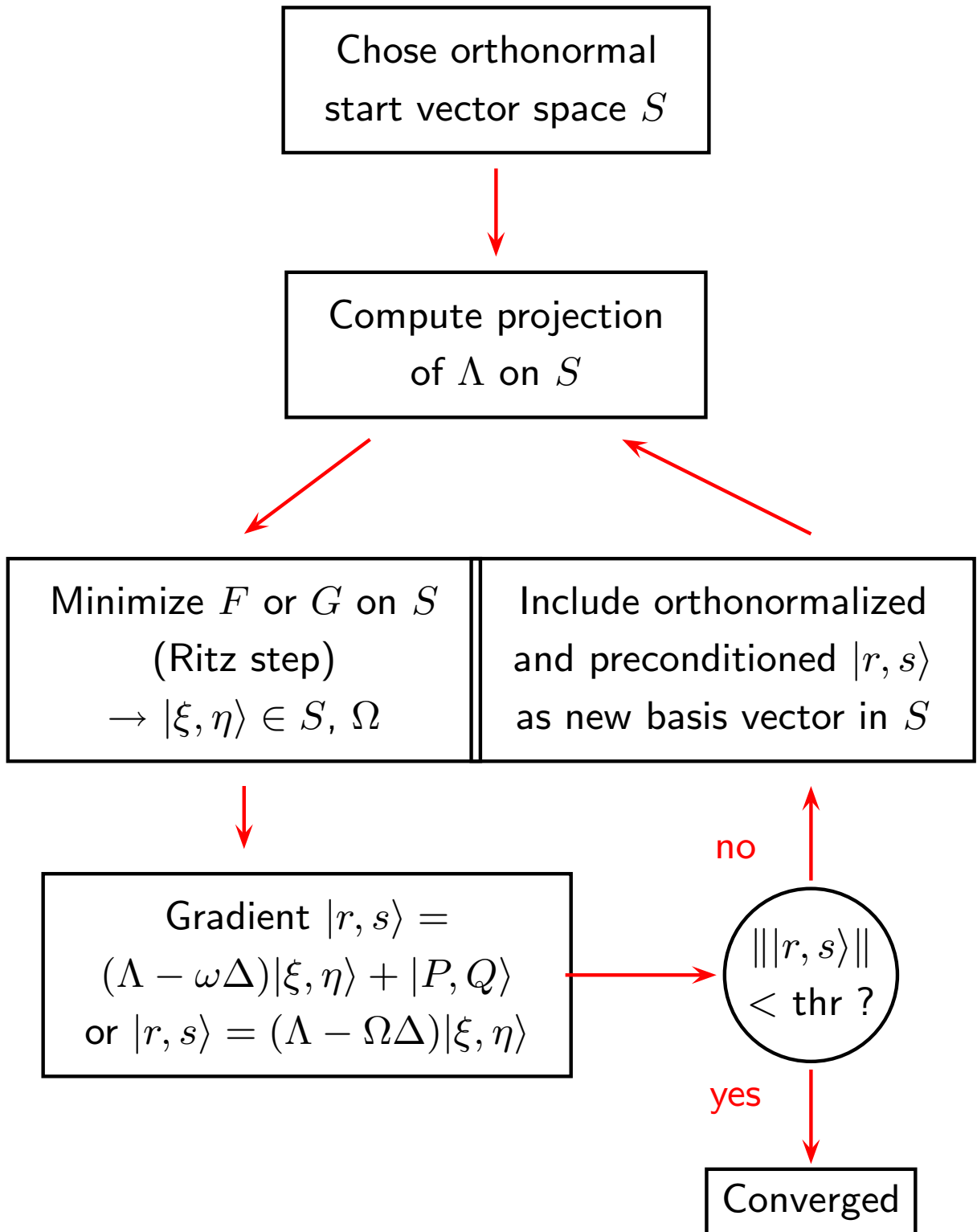
- In most applications, only a small number of perturbations / excited states is of interest
- Minimize the functionals

$$F[X, Y] = \langle X, Y | \Lambda - \omega \Delta | X, Y \rangle + \langle X, Y | P, Q \rangle + \langle P, Q | X, Y \rangle,$$
$$G[X, Y, \Omega] = \langle X, Y | \Lambda | X, Y \rangle - \Omega(\langle X, Y | \Delta | X, Y \rangle - 1)$$

on an iteratively expanded subspace of  $L$

- Requires small number of matrix-vector products  $\Lambda | X, Y \rangle$
- Using these techniques **A** and **B** never need to be set up and stored!
- First proposed by Hestenes, Stiefel, and Lanczos, useful preconditioning by Davidson

# Iterative subspace methods



## Integral direct iterative algorithms I

- Usually less than 10 iterations required for residual norm  $\leq 10^{-5}$
- A posteriori error bounds available
- **Integral direct** algorithm:
  - Transform vectors, not integrals
  - Compute **non-vanishing** integrals “on the fly”, i.e., discard them after use  $\rightarrow$  pre-screening
- Time-determining step: Matrix-vector products

$$|U, V\rangle = \Lambda |X, Y\rangle,$$

best calculated as

$$(U \pm V) = (A \pm B)(X \pm Y)$$

## Integral direct iterative algorithms II

- Transformation MO-AO

$$(X \pm Y)_{\mu\nu\sigma} = \frac{1}{2} \sum_{ia} (X \pm Y)_{ia\sigma} (C_{\mu i\sigma} C_{\nu a\sigma} \pm C_{\mu a\sigma} C_{\nu i\sigma})$$

- Matrix-vector multiplication (AO basis)

$$(U + V)_{\mu\nu\sigma} = \sum_{\kappa\lambda\sigma'} (2(\mu\nu|\kappa\lambda) + 2f_{\mu\nu\sigma\kappa\lambda\sigma'}^{\text{xc}} - c_x \delta_{\sigma\sigma'} [(\mu\kappa|\nu\lambda) + (\mu\lambda|\nu\kappa)]) (X + Y)_{\kappa\lambda\sigma'}$$

$$(U - V)_{\mu\nu\sigma} = \sum_{\kappa\lambda\sigma'} c_x \delta_{\sigma\sigma'} [(\mu\kappa|\nu\lambda) - (\mu\lambda|\nu\kappa)] (X - Y)_{\kappa\lambda\sigma'}$$

- Transformation AO-MO

$$(U \pm V)_{ia\sigma} \rightarrow \frac{1}{2} \sum_{\mu\nu} (U \pm V)_{\mu\nu\sigma} (C_{\mu i\sigma} C_{\nu a\sigma} \pm C_{\mu a\sigma} C_{\nu i\sigma})$$

## Two-electron integrals $(\mu\nu|\kappa\lambda)$

Well-established techniques from **ground-state quantum chemistry**:

- **A priori bound** from Cauchy-Schwarz inequality,

$$|(\mu\nu|\kappa\lambda)| \leq (\mu\nu|\mu\nu)^{1/2}(\kappa\lambda|\kappa\lambda)^{1/2}$$

Result:  $O(N^4) \rightarrow O(N^2)$

- **Analytical expression** for  $(ss|ss)$ , higher  $l$  by analytical **recursion** (Obara-Saika)
- **Auxiliary expansion (RI)** techniques:

$$(\mu\nu|\kappa\lambda) \rightarrow \sum_{pq} (\mu\nu|p)(p|q)^{-1}(q|\kappa\lambda)$$

- Prefactor reduced by 10 – 100
- Efficient for Coulomb only
- More in Dmitrij Rappoport's talk

## Exchange-correlation contributions

$$(U + V)_{\mu\nu\sigma} \rightarrow \sum_{\kappa\lambda\sigma'} f_{\mu\nu\sigma\kappa\lambda\sigma'}^{\text{xc}} (X + Y)_{\kappa\lambda\sigma'}$$

Example: ALDA,

$$E^{\text{xc}}[\rho] = \int d^3r f(\rho_\alpha(\mathbf{r}), \rho_\beta(\mathbf{r}))$$

1. Evaluate “density response” on the grid  $O(N^3) \rightarrow O(N)$

$$\rho^{(1)}(\mathbf{r}_i) = \sum_{\mu\nu} \chi_\mu(\mathbf{r}_i) \chi_\nu(\mathbf{r}_i) (X + Y)_{\mu\nu\sigma}$$

2. Perform quadrature  $O(N^3) \rightarrow O(N)$

$$(U + V)_{\mu\nu\sigma} \rightarrow \sum_i w_i \chi_\mu(\mathbf{r}_i) \chi_\nu(\mathbf{r}_i) \sum_{\sigma'} \frac{\partial^2 f}{\partial \rho_\sigma(\mathbf{r}_i) \partial \rho_{\sigma'}(\mathbf{r}_i)} \rho_{\sigma'}^{(1)}(\mathbf{r}_i)$$

Equivalent to computation of the first order response of the xc *potential!*



## Turbomole implementation *escf*

System	Sym.	Method	$N_{\text{BF}}$	$p^a$	CPU	R <sup>b</sup>
Tris(Alanine)-Co <sup>III</sup>	$C_3$	B3LYP	386	100	12:04	B
Cu-phthalocyanin <sup>c</sup>	$D_{4h}$	B3LYP	706	90	40:24	B
Tetrathia-[7]helicene	$C_2$	B3LYP	482	50	30:13	B
Fullerene C <sub>540</sub>	$I_h$	BP/RI	8100	3	19:17	B
"Cd <sub>10</sub> Se <sub>16</sub> " <sup>d</sup>	$T$	BP/RI	2804	300	128:04	A
Vancomycin	$C_1$	BP/RI	1294	100	46:08	B
Methylcobalamin	$C_1$	BP/RI	1600	100	62:18	A

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<sup>a</sup>number of excited states

<sup>b</sup>platform used. A: 1.2 GHz Athlon PC, B: 440 MHz HP J5000

<sup>c</sup>open shell

<sup>d</sup>Cd<sub>10</sub>Se<sub>4</sub>(SePh)<sub>12</sub>(P<sup>n</sup>Pr<sub>3</sub>)<sub>4</sub>

TURBOMOLE V5-4

Present limit (single processor): 200-1000 atoms

## Excited state properties

- **Problem:** Linear response theory supplies excitation energies and transition moments, but no excited state wavefunction!
- **Solution:** Define excited state properties via the **response of the excited state energy**  $E^{\text{es}}[v]$ .
- Examples:
  - Excited state dipole moments:  $\left. \frac{\partial E^{\text{es}}[v]}{\partial \epsilon} \right|_{\epsilon=0}$
  - Excited state density  $\left. \frac{\delta E^{\text{es}}[v]}{\delta v^{\text{ext}}(\mathbf{r})} \right|_{v^{\text{ext}}(\mathbf{r})=0}$
  - Excited state gradients  $\left. \frac{\partial E^{\text{es}}[v]}{\partial R_\mu} \right|_{R_\mu=0}$
- **WANTED:** Fully variational expression for the excited state energy

## Lagrangian of the excited state energy

- Define Lagrangian

$$L[X, Y, \Omega, C, Z, W] = E_{\text{GS}} + G[X, Y, \Omega] + \sum_{ia} Z_{ia} H_{\text{KS } ia}^{(0)} - \sum_{pq} W_{pq} (S_{pq} - \delta_{pq})$$

- $E_{\text{GS}}$ : Ground state energy functional
  - $S$ : Overlap matrix
  - $Z, W$ : Additional Lagrange multipliers
- Result:
    - The minimum of  $L$  with respect to all parameters is the total energy of the first excited state.

F. F., R. Ahlrichs, *J. Chem. Phys.* **117** (2002), 7433.

## Stationarity conditions

$$(1) \quad \frac{\partial L}{\partial Z_{ia}} = F_{ia} = 0, \quad \frac{\partial L}{\partial W_{pq}} = S_{pq} - \delta_{pq} = 0$$

Ground state KS equations  $\rightarrow$  Molecular orbital coefficients  $C$

$$(2) \quad \frac{\partial L}{\partial \langle X, Y |} = (\Lambda - \Omega \Delta) |X, Y\rangle = 0, \quad \frac{\partial L}{\partial \Omega} = \langle X, Y | \Delta | X, Y\rangle - 1 = 0$$

TDKS eigenvalue problem (Casida's equations)  $\rightarrow$  Excitation energy  $\Omega$ , excitation vector  $|X, Y\rangle$

$$(3) \quad \frac{\partial L}{\partial C} = 0$$

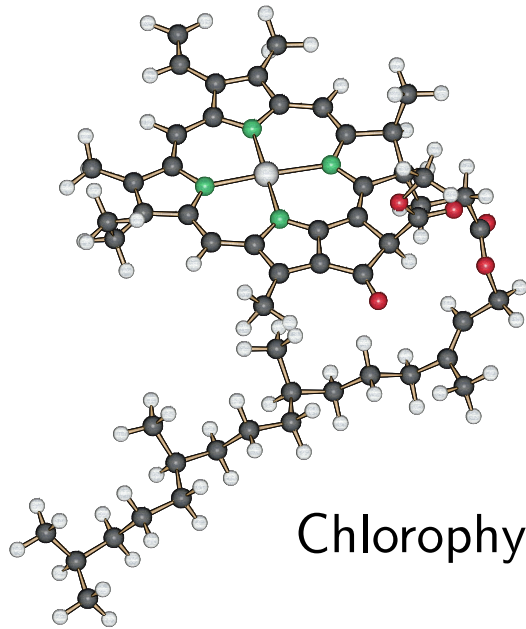
Z vector equation  $(A + B)Z = -R \rightarrow$  relaxed excited state density matrix  $P$ , energy weighted relaxed density matrix  $W$

## Excited state properties

$$L^\xi = \sum_{\mu\nu\sigma} h_{\mu\nu}^\xi P_{\mu\nu\sigma} - \sum_{\mu\nu\sigma} S_{\mu\nu}^\xi W_{\mu\nu\sigma} + \sum_{\mu\nu\kappa\lambda\sigma\sigma'} (\mu\nu|\kappa\lambda)^\xi \Gamma_{\mu\nu\sigma\kappa\lambda\sigma'} \\ + \sum_{\mu\nu\sigma} V_{\mu\nu\sigma}^{\text{xc}(\xi)} P_{\mu\nu\sigma} + \sum_{\mu\nu\kappa\lambda\sigma\sigma'} f_{\mu\nu\sigma\kappa\lambda\sigma'}^{\text{xc}(\xi)} (X+Y)_{\mu\nu\sigma} (X+Y)_{\kappa\lambda\sigma'}$$

- General expression for integral-direct evaluation of excited state first-order properties
- Almost identical to ground state expression  $\rightarrow$  same  $O(N)/O(N^2)$  scaling
- Variational stability of  $L \rightarrow$  **No** MO coefficient derivatives  $C_{\mu\rho\sigma}^\xi$
- The cost for computing excited state gradients analytically is **independent** of the number of nuclear degrees of freedom

## Turbomole implementation: egrad



GS energy	0:33 h
ES energy+grad	1:44 h
opt. cycles	13

TURBOMOLE V5-7, RIDFT/BP-86/SV(P), 1.7 GHz Athlon PC

Excited state geometry optimization is not significantly more expensive than ground state geometry optimization

D. Rappoport, F. F., *J. Chem. Phys.* **122** (2005), 064105.

## Summary: Implementation I

- Basis set expansion reduces TDKS response and eigenvalue problems to finite-dimensional matrix algebra
- Iterative subspace methods:
  - Only two-index quantities (vectors) need to be stored and handled, **no four-index MO integrals**
  - Time-determining steps:  $O(N^2)$ – $O(N)$  scaling, very similar to ground-state Fock matrix construction
  - Significant savings by simultaneous processing of several perturbations/states
  - More efficient than real-time propagation for linear response
- Solving the TDKS response equations / the TDKS eigenvalue problem is *less* expensive than solving the ground state KS equations

## Summary: Implementation II

- Excited state properties are best calculated as analytical derivatives of the excited state Lagrangian
- Analytical derivatives yield exact response of the excited state energy in any basis set
- The cost of analytical excited state gradients does not scale with the number of nuclear degrees of freedom
- Large systems are the domain of TDDFT in quantum chemistry → implementation matters
- Present limit (single processor): 200-1000 atoms

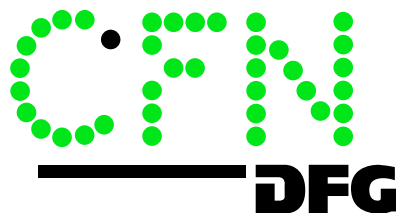


## Further reading

- [1] *Time-dependent density functional theory in quantum chemistry*. F. F. and K. Burke, in *Annual Reports in Computational Chemistry* 1, edited by D. C. Spellmeyer, Elsevier, Amsterdam, 2005, p. 19.
- [2] *Density functional methods for excited states: equilibrium structure and electronic spectra*. F. F. and D. Rappoport, In *Computational Photochemistry*, edited by M. Olivucci, Elsevier, Amsterdam, 2005, p. 93.
- [3] *Time-dependent density functional theory*, edited by M. Marques, C. A. Ullrich, F. Nogueira, A. Rubio, K. Burke, and E. K. U. Gross, Springer, Berlin, 2006.

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