Backflow Sparsity

Pablo López Ríos
27-Jul-2008

Backflow Sparsity

in Slater wave functions

Pablo López Ríos

27-Jul-2008

Taking advantage of

Backflow Sparsity

in Slater wave functions

Pablo López Ríos

27-Jul-2008

Taking advantage of

Backflow Sparsity

in Slater wave functions

(for dummies)

Pablo López Ríos

27-Jul-2008

Backflow

- Backflow'd wave function:

$$\Psi = \Psi_S[\boldsymbol{R} + \boldsymbol{\Xi}(\boldsymbol{R})]\exp[J(\boldsymbol{R})]$$

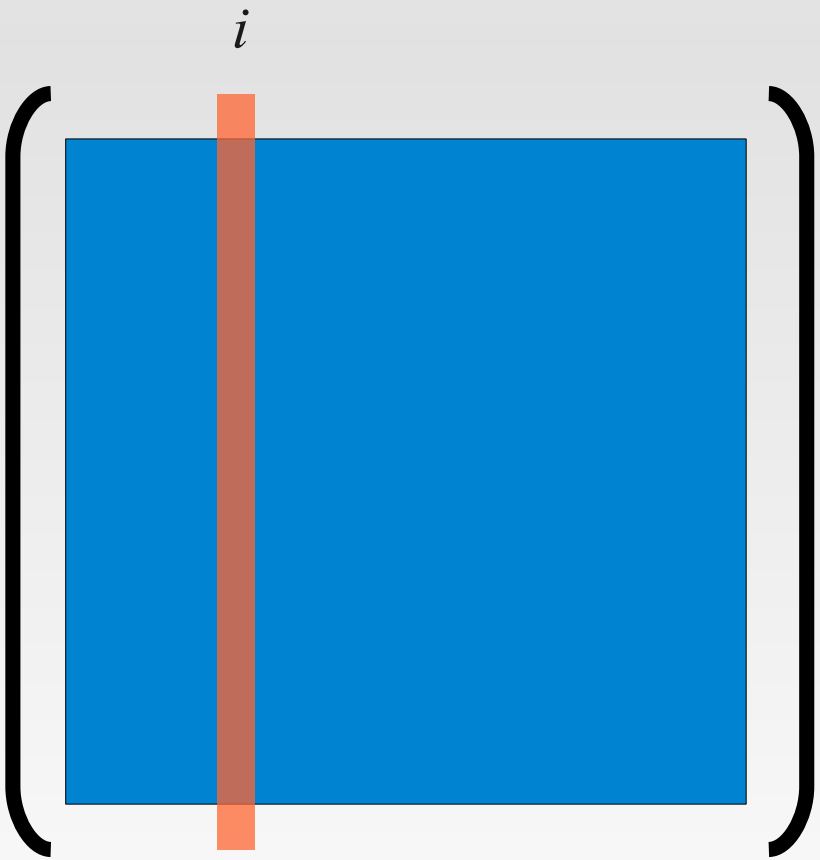
- Backflow displacement $\boldsymbol{\xi}_i = \boldsymbol{\xi}_i^{ee} + \boldsymbol{\xi}_i^{en} + \boldsymbol{\xi}_i^{een} + \ldots$ with:

$$\boldsymbol{\xi}_i^{ee} = \sum_{j \neq i}^{N} \eta(r_{ij})\boldsymbol{r}_{ij} \qquad \boldsymbol{\xi}_i^{en} = \sum_{I}^{N_{ion}} \mu(r_{iI})\boldsymbol{r}_{iI}$$

$$\boldsymbol{\xi}_i^{ee} = \sum_{j \neq i}^{N} \sum_{I}^{N_{ion}} \left[\Phi(r_{ij}, r_{iI}, r_{jI})\boldsymbol{r}_{ij} + \Theta(r_{ij}, r_{iI}, r_{jI})\boldsymbol{r}_{iI}\right]$$

Slater wave function

- One-electron update: Sherman-Morrison formula



$$q = \sum_{p}^{N} \bar{S}_{ip} S'_{pi}$$

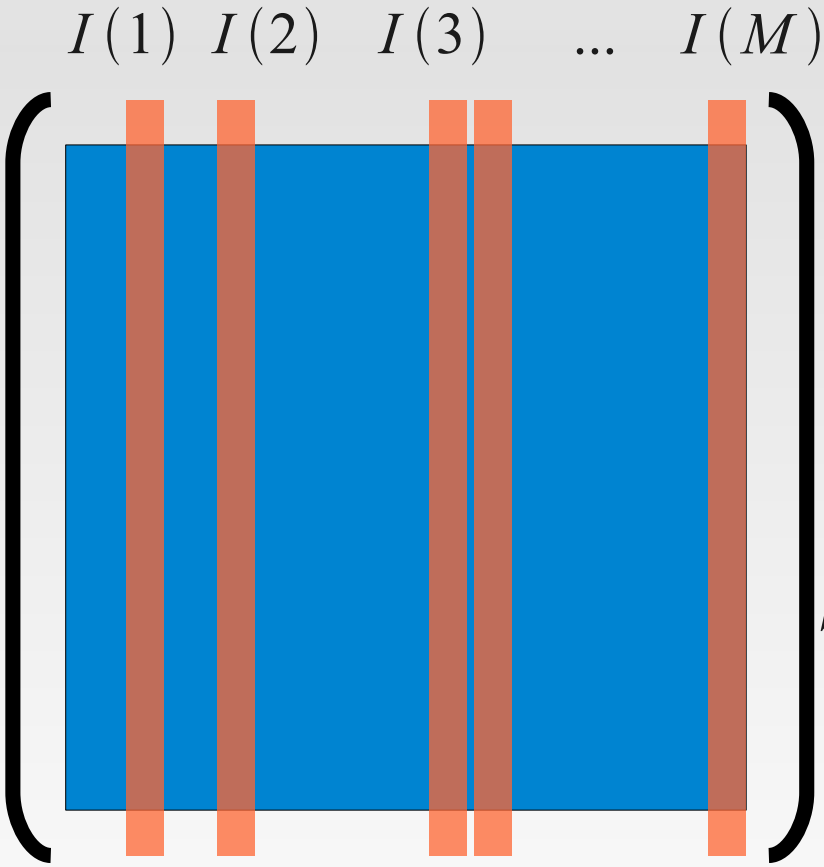
$$det[S'] = q\, det[S]$$

$$\bar{S}'_{kj} = \bar{S}_{kj} - \left(\sum_{p}^{N} \bar{S}_{kp} S'_{pi} \right) q^{-1} \bar{S}_{ij} \qquad (k \neq i)$$

$$\bar{S}'_{ij} = q^{-1} \bar{S}_{ij}$$

Slater-backflow wave function

- One-electron update: Woodbury formula



$$Q_{\alpha\beta} = \sum_{j}^{N} \bar{S}_{I(\alpha)j} S'_{jI(\beta)}$$

$$det[S'] = det[Q]\, det[S]$$

$$\bar{S}'_{kj} = \bar{S}_{kj} - \sum_{\alpha}^{M} \sum_{\beta}^{M} \sum_{p}^{N} \bar{S}_{kp} S'_{pI(\alpha)} \bar{Q}_{\alpha\beta} \bar{S}_{I(\beta)j} \qquad (k \neq I(\gamma))$$

$$\bar{S}'_{I(\gamma)j} = \sum_{\beta}^{M} \bar{Q}_{\gamma\beta} \bar{S}_{I(\beta)j}$$

Cost

- Backflow:
  - Cfg. analysis level 1 n^2
  - Cfg. analysis level 2 nm^2
  - One-part. move analysis nm
  - Transformation nm
  - One-particle transf. update m
  - Grad. (chain rule) m
  - All grads. (chain rule) nm
  - Lap. (chain rule) m^2
  - All laps. (chain rule) nm^2

Cost

- Slater-backflow:
  - Entire matrix $x(n)n^2$
  - Matrix column $x(n)n$
  - Invert matrix n^3
  - Q nm^2
  - Update inverse n^2m
  - Grads. for one particle nm
  - All grads. n^2
  - All laps. n^2m'