A general Jastrow factor

One Jastrow to rule them all...

Early ideas

Pablo López Ríos

27-Jul-2008

Why?

- All Jastrow terms, with the exception of U_{RPA} and W, are constructed in the same manner

- The work required to implement the new Jastrow is compensated by:
  - No need to implement **new terms** (four-body, say)
  - Easy to implement **new functional bases** (other than natural powers)
  - Easy to add **anisotropies** or dependencies on **external potentials**

The current Jastrow terms

- The U term:

$$U = \sum_{i,j}^{N} \bar{\delta}_{ij} f(r_{ij}) \sum_{\mu=0}^{p} \alpha_{\mu}^{P_{ij}} r_{ij}^{\mu}$$

- The χ term:

$$\chi = \sum_{I}^{M} \sum_{i}^{N} f(r_{iI}) \sum_{\nu=0}^{q} \beta_{\nu}^{S_{iI}} r_{iI}^{\nu}$$

- The F term:

$$F = \sum_{I}^{M} \sum_{i,j}^{N} \bar{\delta}_{ij} f(r_{iI}) f(r_{jI}) \sum_{\mu=0}^{p} \sum_{\nu_1,\nu_2=0}^{q} \gamma_{\mu,\nu_1,\nu_2}^{P_{ij},S_{iI},S_{jI}} r_{ij}^{\mu} r_{iI}^{\nu_1} r_{jI}^{\nu_2}$$

A general Jastrow term

$$G_{n,m} = \sum_{\{J(\gamma)\}_{\gamma=1}^{m}}^{M} \sum_{\{I(\alpha)\}_{\alpha=1}^{n}}^{N} \prod_{\alpha \neq \beta}^{n} \bar{\delta}_{I(\alpha) I(\beta)} \prod_{\gamma \neq \lambda}^{m} \bar{\delta}_{J(\gamma) J(\lambda)} \times$$

$$\times \left(\delta_{m0} \prod_{\alpha<\beta}^{n} f\left(r_{I(\alpha) I(\beta)}\right) + \bar{\delta}_{m0} \prod_{\alpha}^{n} \prod_{\gamma}^{m} f\left(r_{I(\alpha) J(\gamma)}\right) \right) \times$$

$$\times \sum_{\{\mu(\alpha,\beta)\}_{\alpha<\beta}^{n}=0}^{p} \sum_{\{\nu(\alpha,\gamma)\}_{\alpha,\gamma}^{n,m}=0}^{q} g_{\{\mu\},\{\nu\}}^{\{P\}\{S\}} \prod_{\alpha<\beta}^{n} \Phi_{\mu(\alpha,\beta)}\left(\underline{r}_{I(\alpha) I(\beta)}\right) \times$$

$$\times \prod_{\alpha}^{n} \prod_{\gamma}^{m} \varphi_{\nu(\alpha,\gamma)}\left(\underline{r}_{I(\alpha) J(\gamma)}\right)$$

- (n,m) = order of the term; (p,q) = expansion orders
- $\Phi_{\mu}(\underline{r})$, $\varphi_{\nu}(\underline{r})$ = basis functions (elec-elec, elec-nuc)
- $\{g\}$ = linear coefficients

Correspondences

- U term:
  - $(n,m)=(2,0)$
  - $f(r)=(r\text{-}L)^C$
  - $\Phi_\mu(\underline{r})=|\underline{r}|^\mu$
- F term:
  - $(n,m)=(2,1)$
  - $f(r)=(r\text{-}L)^C$
  - $\Phi_\mu(\underline{r})=|\underline{r}|^\mu$
  - $\varphi_\nu(\underline{r})=|\underline{r}|^\nu$
- P term:
  - $(n,m)=(2,0)$
  - $\mathrm{f(r)=1}$
  - $\Phi_\mu(\underline{r})=\cos(\underline{G}_\mu\cdot\underline{r})$
- H term:
  - $(n,m)=(3,0)$
  - $f(r)=(1\text{-}r/L)^C$
  - $\Phi_\mu(\underline{r})=|\underline{r}|^\mu$