A General Jastrow Factor

One Jastrow to rule them all,
one Jastrow to bind them.*

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* without the “darkness” stuff

The Jastrow Factor

- Typical QMC trial wave function form: Slater-Jastrow:

$$\Psi_T(\boldsymbol{R}) = e^{J(\boldsymbol{R})} \Psi_S(\boldsymbol{R})$$

- In VMC, Jastrow describes correlations
- In DMC, Jastrow just stabilizes method

The Jastrow Factor

- Jastrow usually sum terms of different rank:

$$J(\boldsymbol{R}) = J_{e-e}(\boldsymbol{R}) + J_{e-n}(\boldsymbol{R}) + J_{e-e-n}(\boldsymbol{R}) + \dots$$

- Each term is expanded on a basis
- Optimizable parameters:
  - Expansion coefficients
  - Internal basis-function parameters

Why Generalize?

- All Jastrow terms constructed the same way
- Work required to implement General Jastrow compensated by:
  - No need to implement **new terms** (e.g., four-body)
  - Easy to implement **new functional bases**
  - Easy to add **anisotropies**
  - Easy to add dependencies on **external potentials**

Current CASINO Jastrow

- The U term:

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

- The χ term:

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

- The F term:

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

General Jastrow Term

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

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

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

- (n,m) = ranks
- (p,q) = exp. orders
- $\Phi_{\mu}(\boldsymbol{r})$ = e-e basis f.
- $\varphi_{\nu}(\boldsymbol{r})$ = e-n basis f.
- $\{g\}$ = linear coeffs
- $\{P\}$ = e-e pair types
- $\{\mu\}$ = e-e pair indices
- $\{S\}$ = e-n pair types
- $\{\nu\}$ = e-n pair indices

Correspondences

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

More Sophisticated Terms

- Dot products:
  - $\Phi_x(\boldsymbol{r})=\hat{\boldsymbol{u}}_x\cdot\boldsymbol{r}$
  - Appropriate constraints on g
- Possibly other interesting ones too

The CASINO Data Format

- parameters.cdf:

```
JASTROW:
  title: Jastrow for a homogeneous electron gas
  term 1:
    rank: [ 2, 0 ]
    e-e-basis: [ type: polynomial, order: 4 ]
    e-e-cutoff: [ type: polynomial ]
    parameters:
      spin-independent:
        rules: [ 1-1 = 2-2, 1-1 = 1-2 ]
        channel 1:
          L: [ 10.d0, optimizable,
               limits: [ 1.d-8, none ] ]
      spin-split:
        rules: [ 1-1 = 2-2 ]
        channel 1:
          model: 1-1
          c_1: [ 0.d0, optimizable ]
          c_2: [ 0.d0, optimizable ]
          c_3: [ 0.d0, optimizable ]
          c_4: [ 0.d0, optimizable ]
        channel 2:
```

General backflow

- Slater-Jastrow-backflow trial wave function:

$$\Psi_T(\boldsymbol{R}) = e^{J(\boldsymbol{R})}\Psi_S[\boldsymbol{X}(\boldsymbol{R})]$$

- with

$$\boldsymbol{x}_i(\boldsymbol{R}) = \boldsymbol{r}_i + \boldsymbol{\xi}_i(\boldsymbol{R})$$

- with

$$\boldsymbol{\xi}_i(\boldsymbol{R}) = \boldsymbol{\xi}_i^{e-e}(\boldsymbol{R}) + \boldsymbol{\xi}_i^{e-n}(\boldsymbol{R}) + \boldsymbol{\xi}_i^{e-e-n}(\boldsymbol{R}) + \ldots$$

- Same approach is possible