A general backflow transformation

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October 7, 2009

Quantum Monte Carlo

The Schrödinger equation for an electronic system

$$\left[\frac{1}{2}\sum_i \nabla_i^2 + \sum_{i<j}\frac{1}{|\mathbf{r}_i-\mathbf{r}_j|} - \sum_I\sum_i \frac{Z_I}{|\mathbf{r}_i-\mathbf{R}_I|}\right]\Phi_0(\mathbf{R}) = E_0\Phi_0(\mathbf{R})$$

- Solvable exactly for very few systems.
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Variational Monte Carlo

Variational estimate of the energy

$$E_0 \leq E_{\mathrm{V}}[\Psi] = \frac{\int \Psi(\mathbf{R})\hat{H}(\mathbf{R})\Psi(\mathbf{R})d\mathbf{R}}{\int \Psi^2(\mathbf{R})d\mathbf{R}} \approx$$

$$\approx \frac{1}{M}\sum_{m;\ \Psi^2}^{M} \frac{\hat{H}(\mathbf{R}_m)\Psi(\mathbf{R}_m)}{\Psi(\mathbf{R}_m)} = E_{\mathrm{VMC}}[\Psi]$$

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- is a very simple method
- along with the variational principle, allows for optimization of a parametrized $\Psi(\mathbf{R};\alpha)$
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The time-dependent Schrödinger equation

$$\hat{H}\Phi(\mathbf{R},t) = i\frac{\partial\Phi(\mathbf{R},t)}{\partial t}$$

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In imaginary time $\tau = it$, with energy shift E_T

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Application:

- Set $\Phi(\mathbf{R},0) = \Psi(\mathbf{R})$.
- $\lim_{\tau\to\infty} \Phi(\mathbf{R},\tau) = \Phi_0(\mathbf{R})$.
- DMC projects out $\Phi_0(\mathbf{R})$ as $\tau \to \infty$.
- Implementation: ensemble of configurations subjected to drift+diffusion+branching in a discretized timeline.

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The Slater-Jastrow wave function

$$\Psi(\mathbf{R}) = \exp\left[J(\mathbf{R})\right] \Psi_S(\mathbf{R})$$

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$$J(\mathbf{R}) = J_{\mathrm{e-e}}(\mathbf{R}) + J_{\mathrm{e-N}}(\mathbf{R}) + J_{\mathrm{e-e-N}}(\mathbf{R}) + \dots$$

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Fixed-form Jastrow factor terms

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$$J_{\mathrm{e-e}}(\mathbf{R}) = \sum_{i<j}^{M} f(r_{ij}) \sum_{\nu}^{p} \lambda_{\nu}^{P_{ij}} r_{ij}^{\nu}$$

$$J_{\mathrm{e-N}}(\mathbf{R}) = \sum_{i}^{N} \sum_{I}^{M} f(r_{iI}) \sum_{\mu}^{q} \lambda_{\mu}^{S_{iI}} r_{iI}^{\mu}$$

$$J_{\mathrm{e-e-N}}(\mathbf{R}) = \sum_{i<j}^{N} \sum_{I}^{M} f(r_{iI}) f(r_{jI}) \sum_{\nu_{ij}}^{p} \sum_{\mu_{iI}\mu_{jI}}^{q} \lambda_{\nu_{ij}\mu_{iI}\mu_{jI}}^{P_{ij}S_{iI}S_{jI}} r_{ij}^{\nu_{ij}} r_{iI}^{\mu_{iI}} r_{jI}^{\mu_{jI}}$$

General Jastrow factor

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$$J_{n,m}(\mathbf{R}) = \sum_{i_1<\ldots<i_n}^{N} \sum_{I_1<\ldots<I_m}^{M} \sum_{\{\nu_{i_\alpha i_\beta}\}_{\alpha<\beta}^{n}}^{p} \sum_{\{\mu_{i_\alpha I_\gamma}\}_{\alpha=1,\gamma=1}^{\alpha=n,\gamma=m}}^{q} \lambda_{\{\nu\}\{\mu\}}^{\{P\}\{S\}} \times \left(\prod_{\alpha<\beta}^{n} \Phi_{\nu_{i_\alpha i_\beta}}^{P_{\sigma(i_\alpha)\sigma(i_\beta)}}(\mathbf{r}_{i_\alpha i_\beta}) \right) \left(\prod_{\alpha}^{n} \prod_{\gamma}^{m} \Theta_{\mu_{i_\alpha I_\gamma}}^{S_{\sigma(i_\alpha)I_\gamma}}(\mathbf{r}_{i_\alpha I_\gamma}) \right)$$

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$$\boldsymbol{\xi}^i_{\mathrm{e-e}}(\mathbf{R}) = \sum_{j\neq i}^{M} f(r_{ij}) \sum_{\nu}^{p} \lambda_\nu^{P_{ij}} r_{ij}^\nu \mathbf{r}_{ij}$$

$$\boldsymbol{\xi}^i_{\mathrm{e-N}}(\mathbf{R}) = \sum_{I}^{M} f(r_{iI}) \sum_{\mu}^{q} \omega_\mu^{S_{iI}} r_{iI}^\mu \mathbf{r}_{iI}$$

$$\begin{aligned}\boldsymbol{\xi}^i_{\mathrm{e-e-N}}(\mathbf{R}) &= \sum_{j\neq i}^{N}\sum_{I}^{M} f(r_{iI}) f(r_{jI}) \sum_{\nu_{ij}}^{p} \sum_{\mu_{iI}\mu_{jI}}^{q} \Big[\lambda^{P_{ij}S_{iI}S_{jI}}_{\nu_{ij}\mu_{iI}\mu_{jI}} r_{ij}^{\nu} r_{iI}^{\mu_{iI}} r_{jI}^{\mu_{jI}} \mathbf{r}_{ij} + \\ &+ \omega^{P_{ij}S_{iI}S_{jI}}_{\nu_{ij}\mu_{iI}\mu_{jI}} r_{ij}^{\nu} r_{iI}^{\mu_{iI}} r_{jI}^{\mu_{jI}} \mathbf{r}_{iI} \Big]\end{aligned}$$

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$$\xi^{i}_{n,m}(\mathbf{R}) = \sum_{i_2<\ldots<i_n}^{N} \sum_{I_1<\ldots<I_m}^{M} \sum_{\{\nu_{i_\alpha i_\beta}\}_{\alpha<\beta}^{n}}^{p} \sum_{\{\mu_{i_\alpha I_\gamma}\}_{\alpha=1,\gamma=1}^{\alpha=n,\gamma=m}}^{q} \times$$

$$\left[\sum_{k=2}^{N} {}^{[ik]}_{\lambda}{}^{\{P\}\{S\}}_{\{\nu\}\{\mu\}} \left(\prod_{\alpha<\beta}^{n} {}^{[ik]}_{\Phi}{}^{P_{\sigma(i_\alpha)\sigma(i_\beta)}}_{\nu_{i_\alpha i_\beta}} (\mathbf{r}_{i_\alpha i_\beta}) \right) \left(\prod_{\alpha}^{n} \prod_{\gamma}^{m} {}^{[ik]}_{\Theta}{}^{S_{\sigma(i_\alpha)I_\gamma}}_{\mu_{i_\alpha I_\gamma}} (\mathbf{r}_{i_\alpha I_\gamma}) \right) \mathbf{r}_{ik} + \right.$$

$$\left. \sum_{K=2}^{N} {}^{[iK]}_{\omega}{}^{\{P\}\{S\}}_{\{\nu\}\{\mu\}} \left(\prod_{\alpha<\beta}^{n} {}^{[iK]}_{\Delta}{}^{P_{\sigma(i_\alpha)\sigma(i_\beta)}}_{\nu_{i_\alpha i_\beta}} (\mathbf{r}_{i_\alpha i_\beta}) \right) \left(\prod_{\alpha}^{n} \prod_{\gamma}^{m} {}^{[iK]}_{\Lambda}{}^{S_{\sigma(i_\alpha)I_\gamma}}_{\mu_{i_\alpha I_\gamma}} (\mathbf{r}_{i_\alpha I_\gamma}) \right) \mathbf{r}_{iK} \right]$$

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