A general backflow transformation

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Quantum Monte Carlo

The Schrödinger equation for an electronic system

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\left[ \frac{1}{2} \sum_i \nabla_i^2 + \sum_{i<j} \frac{1}{|r_i - r_j|} - \sum_I \sum_i \frac{Z_I}{|r_i - R_I|} \right] \Phi_0(R) = E_0 \Phi_0(R)
\]

- Solvable exactly for very few systems.
- In general we don’t know the exact \( \Phi_0(R) \).
- We can give an approximate \( \Psi(R) \) instead.
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Variational Monte Carlo

Variational estimate of the energy

$$E_0 \leq E_V[\Psi] = \frac{\int \psi(R)\hat{H}(R)\psi(R)dR}{\int \psi^2(R)dR} \approx \frac{1}{M} \sum_{m}^{M} \frac{\hat{H}(R_m)\psi(R_m)}{\psi(R_m)} = E_{VMC}[\Psi]$$

The VMC method:
- is a very simple method
- along with the variational principle, allows for optimization of a parametrized $\Psi(R; \alpha)$
- is entirely dependent on the quality of $\Psi(R)$
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Diffusion Monte Carlo

The time-dependent Schrödinger equation

\[ \hat{H} \Phi(R, t) = i \frac{\partial \Phi(R, t)}{\partial t} \]

\[ \Phi(R, t) = \sum_{n} c_n \Phi_n(R) e^{-i E_n t} \]

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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- is a more complicated, expensive method
- is a more accurate method
- (for fermions) only depends on the quality of the nodes of $\psi(\mathbf{R})$ (nodes $\equiv$ region where $\psi(\mathbf{R}) = 0$).
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The Jastrow factor

The Slater-Jastrow wave function

\[ \psi(\mathbf{R}) = \exp[J(\mathbf{R})] \psi_s(\mathbf{R}) \]

The Jastrow factor:

- is a compact parametrization to describe electronic correlation
- does not change the nodes of the wave function, thus leaving the DMC energy unchanged
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The Slater-Jastrow-backflow wave function

\[ \psi(R) = \exp[J(R)] \psi_S[X(R)] \]

The backflow transformation

\[ x_i(R) = r_i + \xi_i(R) \]

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Fixed-form Jastrow factor terms

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

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

\[
J_{e-e-N}(R) = \sum_{i<j}^N \sum_{I}^M f(r_{iI}) f(r_{jI}) \sum_{\nu_{ij}}^p \sum_{\mu_{iI} \mu_{jI}}^q \lambda_{\nu_{ij} \mu_{iI} \mu_{jI}}^{P_{ij} S_{iI} S_{jI}} r_{ij}^{\nu_{ij}} r_{iI}^{\mu_{iI}} r_{jI}^{\mu_{jI}}
\]
General Jastrow factor

\[ J_{n,m}(\mathbf{R}) = \sum_{i_1<...<i_n}^{N} \sum_{I_1<...<I_m}^{M} \sum_{\nu_{i_\alpha i_\beta}}^{p} \sum_{\mu_{i_\alpha I_\gamma}}^{q} \lambda_{\{P\}\{S\}}^{\{\nu\}\{\mu\}} \times \]

\[
\left( \prod_{\alpha<\beta}^{n} \phi_{\nu_{i_\alpha i_\beta}}(\mathbf{r}_{i_\alpha i_\beta}) \right) \left( \prod_{\alpha}^{n} \prod_{\gamma}^{m} \Theta_{\mu_{i_\alpha I_\gamma}}(\mathbf{r}_{i_\alpha I_\gamma}) \right)
\]
Fixed-form backflow terms

\[ \xi_e^{i} (R) = \sum_{j \neq i}^{M} f(r_{ij}) \sum_{\nu}^{p} \lambda_{\nu} P_{ij} r_{ij} \]

\[ \xi_{e-N}^{i} (R) = \sum_{I}^{M} f(r_{iI}) \sum_{\mu}^{q} \omega_{\mu} S_{iI} r_{iI} \]

\[ \xi_{e-e-N}^{i} (R) = \sum_{j \neq i}^{N} \sum_{I}^{M} f(r_{iI}) f(r_{jI}) \sum_{\nu_{ij}}^{p} \sum_{\mu_{il} \mu_{jI}}^{q} \left[ \lambda_{\nu_{ij} \mu_{il} \mu_{jI}} r_{ij} r_{iI} r_{jI} r_{ij} + \omega_{\nu_{ij} \mu_{il} \mu_{jI}} S_{iI} S_{jI} r_{ij} r_{iI} r_{jI} + \right] \]
General backflow transformation

\[ \xi^{i}_{n,m}(R) = \sum_{i_2 < \ldots < i_n}^{N} \sum_{I_1 < \ldots < I_m}^{M} \sum_{\alpha < \beta}^{p} \sum_{\gamma \alpha}^{q} \times \]

\[ \left[ \sum_{k=2}^{N} \left[ iK \right] \left\{ P \right\} \left\{ S \right\} \left( \prod_{\alpha < \beta}^{n} \left[ iK \right] \right) \left( \prod_{\gamma}^{m} \left[ \right] \right) S_{\sigma(\alpha)\gamma}^{i\alpha} (r_{i\alpha i\gamma}) \right] \left( r_{ik} \right) \]

\[ + \sum_{K=2}^{N} \left[ iK \right] \left\{ P \right\} \left\{ S \right\} \left( \prod_{\Delta}^{n} \left[ iK \right] \right) \left( \prod_{\gamma}^{m} \left[ \right] \right) S_{\sigma(\alpha)\gamma}^{i\alpha} (r_{i\alpha i\gamma}) \left( r_{iK} \right) \]
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