Quantum Monte-Carlo Studies of Generalized Many-body Systems

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Contents

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&= \sum_k C_k \exp(-(E_k - E_0)\tau)\,|\Psi_k\rangle \\
&= C_0\,|\Psi_0\rangle + \sum_{k=1} C_k \exp(-\Delta E_k \tau)\,|\Psi_k\rangle\,,
\end{aligned}$$

where $\Delta E_k > 0$ and $C_k = \langle \Psi_k | \Psi_T \rangle$.

In other words

$$\lim_{\tau\to\infty} \langle \mathbf{r}| \widehat{\mathbf{P}}(\tau) |\Psi_T\rangle = \langle \Psi_0|\Psi_T\rangle \, \Psi_0(\mathbf{r}). \tag{1}$$

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Solution: Introduce a *trial energy* $E_T(\tau)$. Will work as long as the trial energy drops below E_1 at a certain stage (and stays there).

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This is achieved by using the following property of the projection operator

$$\begin{aligned}\widehat{\mathbf{P}}(\tau+\delta\tau) &= \exp(-(\widehat{\mathbf{H}} - E_T(\tau+\delta\tau))(\tau+\delta\tau)) \\ &= \exp(-(\widehat{\mathbf{H}} - E_T(\tau+\delta\tau))\delta\tau) \\ &\quad \times \exp(-(\widehat{\mathbf{H}} - E_T(\tau+\delta\tau))\tau) \\ &\simeq \exp(-(\widehat{\mathbf{H}} - E_T(\tau+\delta\tau))\delta\tau)\widehat{\mathbf{P}}(\tau),\end{aligned}$$

where the relation is approximate due to E_T not being constant.

Let $|\Phi(\tau)\rangle$ represent $\widehat{\mathbf{P}}(\tau)\,|\Psi_T\rangle$. Using the relation from the previous slide reveals

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\end{aligned}$$

where $\langle \mathbf{r} |\, \exp(-(\widehat{\mathbf{H}} - E_T)\delta\tau)\, | \mathbf{r}' \rangle \equiv G(\mathbf{r}', \mathbf{r}; \delta\tau)$ is a *Green's function* interpreted as the transition probability between $\mathbf{r}$ and $\mathbf{r}'$.

Idea: In order to relate the Green's function to well known Markov processes, the exponential is split

$$\begin{aligned}\exp(-(\widehat{\mathbf{H}} - E_T)\delta\tau) &= \exp\left(\frac{1}{2}\nabla^2\delta\tau - (\widehat{\mathbf{V}} - E_T)\delta\tau\right) \\ &= \exp\left(\frac{1}{2}\nabla^2\delta\tau\right)\exp(-(\widehat{\mathbf{V}} - E_T)\delta\tau) \\ &\quad + \mathcal{O}(\delta\tau^2),\end{aligned}$$

where the kinetic part describes a diffusion process with diffusion constant $D = \frac{1}{2}$, and the potential part describes a weighting (linear in position space). This is referred to as the *short time approximation*.

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Solution: By evolving $f(\mathbf{r}, \tau) = \Phi(\mathbf{r}, \tau)\Psi_T(\mathbf{r})$ instead of $\Phi(\mathbf{r}, \tau)$ alone, the singularities are *implicitly* taken care of.

Originally:

$$\frac{\partial \Phi(\mathbf{r},\tau)}{\partial \tau} = \left[\frac{1}{2}\nabla^2 - \left(\widehat{\mathbf{V}} - E_T\right)\right]\Phi(\mathbf{r},\tau).$$

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Importance sampled:

$$\frac{\partial f(\mathbf{r},\tau)}{\partial \tau} = \left[\frac{1}{2}\nabla\cdot(\nabla - \mathbf{F}(\mathbf{r})) - (E_L(\mathbf{r}) - E_T)\right] f(\mathbf{r},\tau), \quad (2)$$

where

$$\mathbf{F}(\mathbf{r}) = 2\Psi_T(\mathbf{r})^{-1}\nabla\Psi_T(\mathbf{r}) \quad (3)$$

is the *quantum force* and

$$E_L(\mathbf{r}) = \Psi_T(\mathbf{r})^{-1}\widehat{\mathbf{H}}\Psi_T(\mathbf{r}) \quad (4)$$

is the *local energy*.

The Green's functions have closed form solutions on the form

$$G_{\text{Diff}}(\mathbf{r}', \mathbf{r}; \delta\tau) \propto \exp\left(-\left|\mathbf{r} - \mathbf{r}' - D\delta\tau\mathbf{F}(\mathbf{r})\right|^2 / 4D\delta\tau\right),$$

$$G_{\text{B}}(\mathbf{r}', \mathbf{r}; \delta\tau) \propto \exp\left(-\left(\frac{1}{2}\left[E_L(\mathbf{r}) + E_L(\mathbf{r}')\right] - E_T\right)\delta\tau\right),$$

where B denotes *branching*.

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This is done by introducing the *Jastrow factor* in $\Psi_T(\mathbf{r})$

$$J(\mathbf{r}) = \prod_{i>j}^{N} \exp\left(a_{ij}\frac{r_{ij}}{1+\beta r_{ij}}\right), \tag{5}$$

where $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$, N is the number of particles, β is a variational parameter, and a_{ij} is a constant depending on the spin eigenvalues of particles i and j.

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The Jastrow factor is tailored to cancel the singularities in the electron-electron Coulomb interaction as the relative distances decrease.

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Idea: The process of projection is modelled by letting an ensemble of walkers span $f(\mathbf{r}, \tau)$. An iteration involves diffusing all the walkers and distributing new weights.

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Solution: By *fixing* the nodes of $f(\mathbf{r}, \tau)$ to match those of $\Psi_T(\mathbf{r})$, the nodes of $\Phi(\mathbf{r}, \tau)$ will consequently match these as well. This is known as the *fixed node approximation* (FNA).

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Consequence: If the FNA is not redundant, $\Phi(\mathbf{r}, \tau)$ will never converge to the exact ground state.

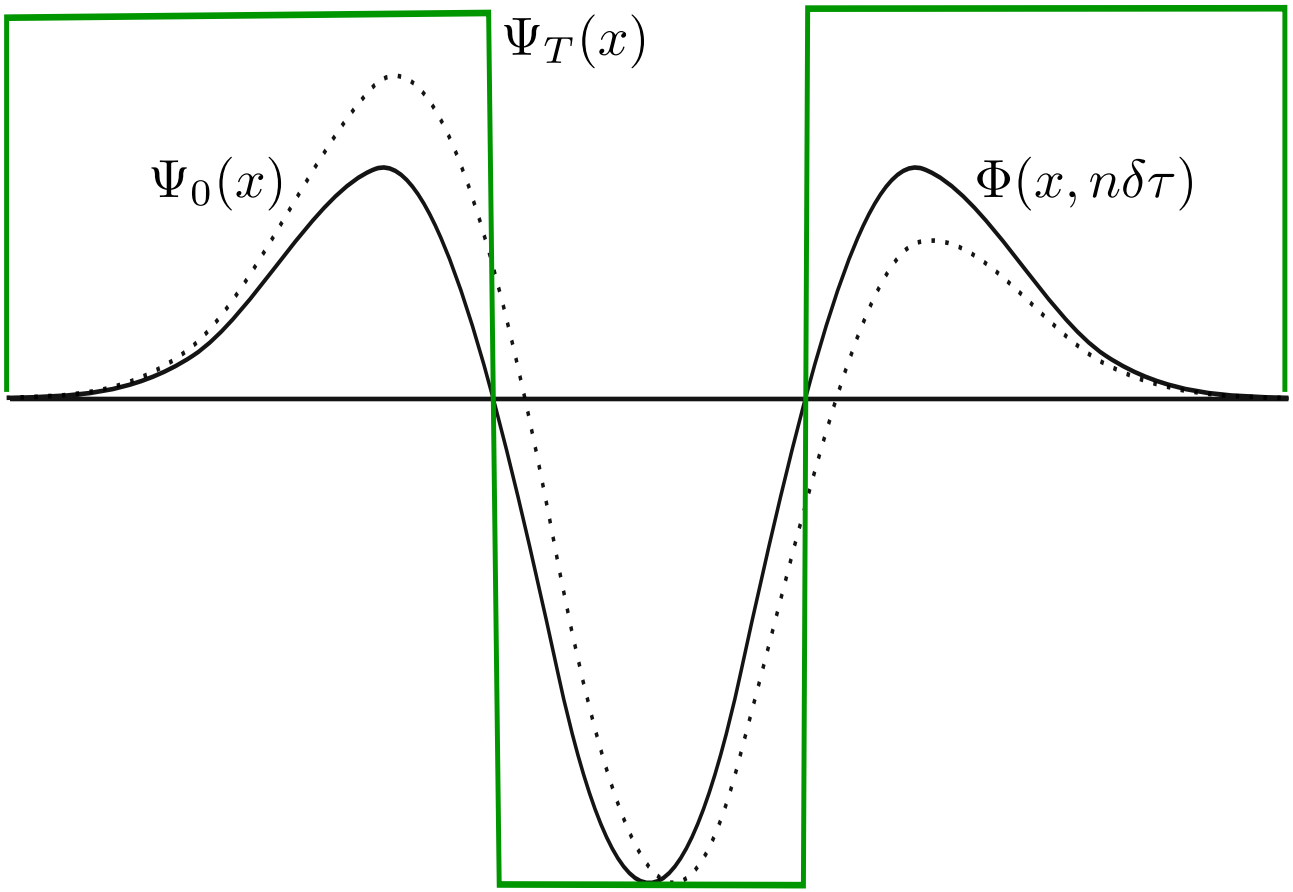

Figure: The fixed node approximation illustrated. The nodes of $\Phi(x, n\delta\tau)$ is fixed to match those of $\Psi_T(x)$.

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Or more compact: Create

$$\overline{G}_{\mathrm{B}} = \mathrm{floor}(G_{\mathrm{B}} + a) \tag{6}$$

copies, where $a \in [0, 1)$ is a uniformly distributed random number. If the value is zero, the walker dies.

Branching

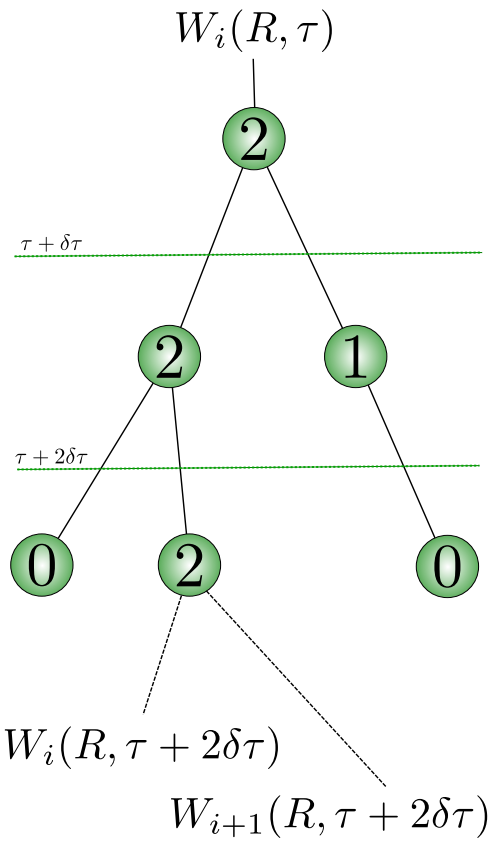

Figure: Branching illustrated. The integer values represent $\overline{G}_{\mathrm{B}}$.

Diffusion

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According to the Fokker-Planck formalism, a new position $\mathbf{r}_{i+1}$ is calculated from the old one, $\mathbf{r}_i$, as follows

$$\mathbf{r}_{i+1} = \mathbf{r}_i + D\delta\tau\mathbf{F}(\mathbf{r}_i) + \xi, \tag{7}$$

where ξ is a vector of normal distributed random numbers with variance $\sqrt{2D\delta\tau}$.

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Solution: The *Metropolis algorithm* will correct this bias:

$$A(i \rightarrow j) = \min\{R_G(i \rightarrow j)R_\psi(i \rightarrow j)^2, 1\}, \tag{8}$$

where $i \rightarrow j$ denotes a transition from state i to state j, A is the probability of accepting the transition,

$$R_G(i \rightarrow j) = G_{\text{Diff}}(\mathbf{r}_j, \mathbf{r}_i; \delta\tau)/G_{\text{Diff}}(\mathbf{r}_i, \mathbf{r}_j; \delta\tau),$$

and

$$R_\psi(i \rightarrow j) = |\Psi_T(\mathbf{r}_j)/\Psi_T(\mathbf{r}_i)|.$$

Recap

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Recap

- The projection process is approximated by the diffusion of an ensemble of walkers with distributed weights.
- Diffusion by the Fokker-Planck equation ensures efficient sampling by the use of the quantum force.
- The Metropolis algorithm corrects the bias introduced by a finite step length. Ensures that the walkers follow $|\Psi_T(\mathbf{r})|^2$.
- After each diffusion step, the walker is either killed or cloned based on the value of the branching Green's function. This ensures that the distribution of walkers follows $f(\mathbf{r}, \tau)$ and not $|\Psi_T(\mathbf{r})|^2$.

Variational Monte-Carlo

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Corresponds to calculating $\langle \Psi_T | \widehat{\mathbf{H}} | \Psi_T \rangle$ using a standard Monte-Carlo approach

$$\langle \Psi_T | \widehat{\mathbf{H}} | \Psi_T \rangle = \int_{\mathbf{r}} |\Psi_T(\mathbf{r})|^2 E_L(\mathbf{r}) \mathrm{d}\mathbf{r} \simeq \frac{1}{N} \sum_{i=1}^{N} \frac{1}{\Psi_T(\mathbf{r_i})} \widehat{\mathbf{H}} \Psi_T(\mathbf{r}_i) \quad (9)$$

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Notice that using any other distribution than $|\Psi_T(\mathbf{r})|^2$ to sample the points $\mathbf{r}_i$ results in undefined samples of the local energy.

Variational Monte-Carlo

Variational Monte-Carlo will always result in an energy which is greater or equal to the exact ground state energy

$$\begin{aligned}
\langle \Psi_T | \hat{\mathbf{H}} | \Psi_T \rangle &= \sum_{ij} C_i^* C_j \underbrace{\langle \Psi_i | \hat{\mathbf{H}} | \Psi_j \rangle}_{E_i \delta_{ij}} \\
&= \sum_i |C_i|^2 E_i \\
&= \sum_i |C_i|^2 (E_0 + \Delta E_i) \\
&= E_0 \underbrace{\sum_i |C_i|^2}_{1} + \underbrace{\sum_i |C_i|^2 \Delta E_i}_{\geq 0} \\
&\geq E_0.
\end{aligned}$$

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The *spatial* wave function is modelled as a single *Slater determinant*, which can be split into two parts $|\mathbf{S}(\mathbf{r})^{\uparrow}|$ and $|\mathbf{S}(\mathbf{r})^{\downarrow}|$ corresponding to two spin levels due to the fact that the Hamiltonian is assumed to be *spin independent*.

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Introducing the variational parameter α into the spatial wave function yields

$$\Psi_T(\mathbf{r};\alpha,\beta) = |\mathbf{S}(\mathbf{r};\alpha)^{\uparrow}||\mathbf{S}(\mathbf{r};\alpha)^{\downarrow}|J(\mathbf{r};\beta) \tag{10}$$

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which upon convergence of the projection results in $\widehat{\mathbf{H}}\,|\Phi(\tau)\rangle = E_0\,|\Phi(\tau)\rangle$. The energy becomes

$$E_{\mathrm{DMC}} = \frac{\langle\Phi(\tau)|\,E_0\,|\Psi_T\rangle}{\langle\Phi(\tau)|\Psi_T\rangle} = E_0. \tag{12}$$

Limitations: VMC

VMC is extremely robust, however, extremely dependent on a good ansatz for $\Psi_T(\mathbf{r})$.

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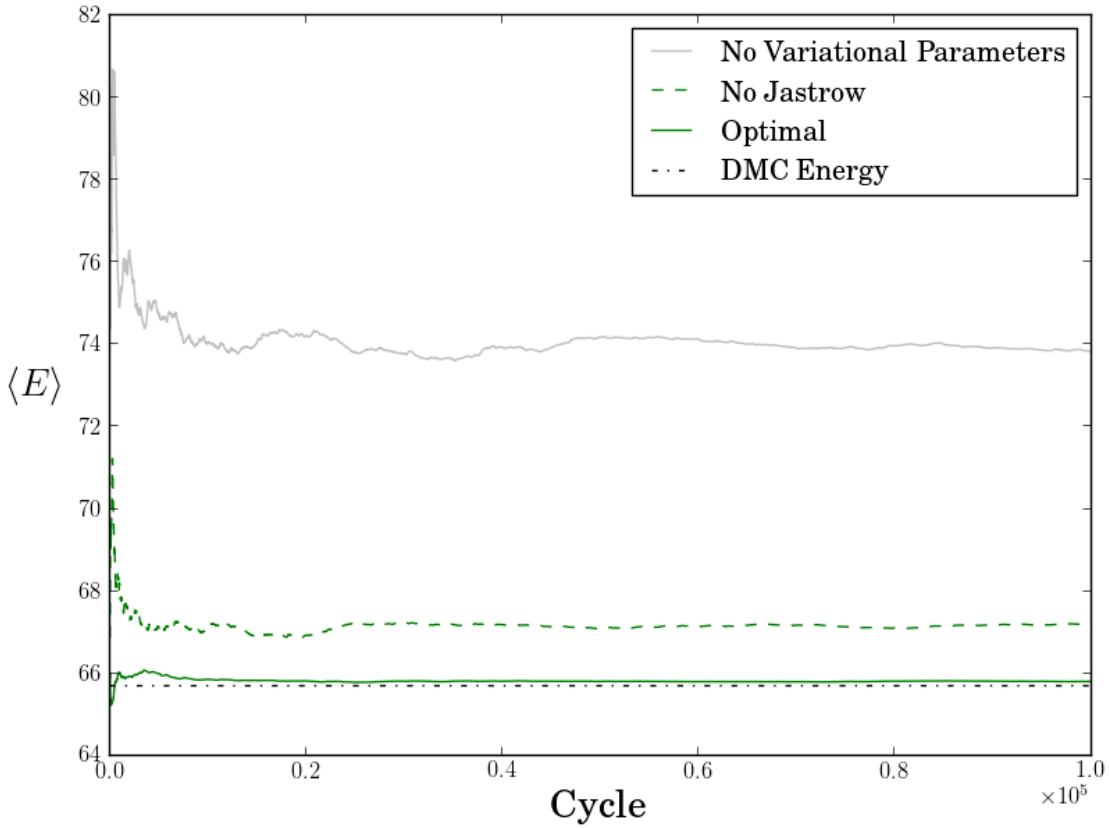

Figure: Comparison of different trial wave functions for a two-dimensional 12-particle quantum dot with unit frequency.

Limitations: DMC

As discussed previously: The fixed node approximation.

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Solution: Can be countered by choosing a lower time step.

Consequence: Slower convergence. Breaking the requirement of *ergodicity*.

Limitations: DMC

Diffusion Monte-Carlo is not as dependent on the trial wave function as VMC.

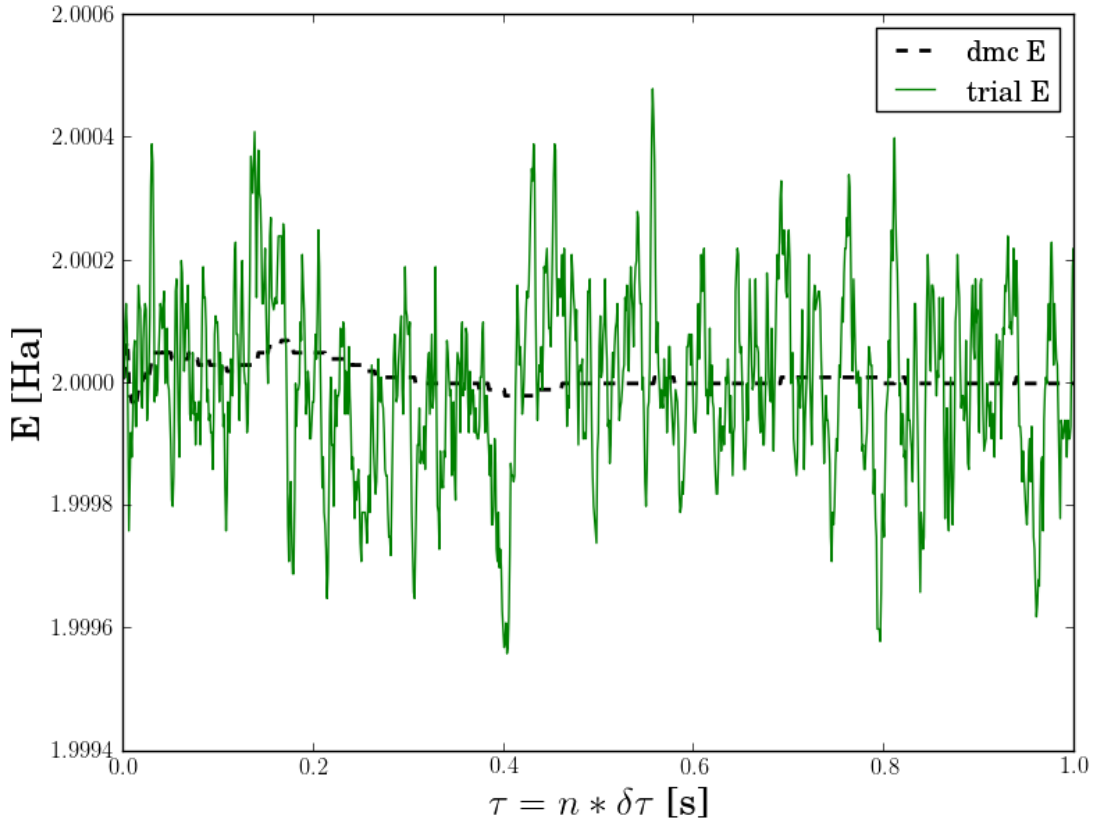

Figure: DMC calculation without the exact wave function. The exact result is $E_0 = 2$. The VMC energy is 2.0042(3), whereas the DMC energy is 2.00000(2).

End of section.

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