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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Problem: Requires a priori knowledge of the exact ground state energy E_0.

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 Markow 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 desribes 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*.

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.

Branching

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Solution: Create $\mathrm{floor}(G_{\mathrm{B}})$ copies with a $G_{\mathrm{B}} - \mathrm{floor}(G_{\mathrm{B}})$ chance of creating an additional copy.

Or more compact: Create

$$\overline{G}_{\mathrm{B}} = \mathrm{floor}(G_{\mathrm{B}} + a) \tag{5}$$

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

Branching

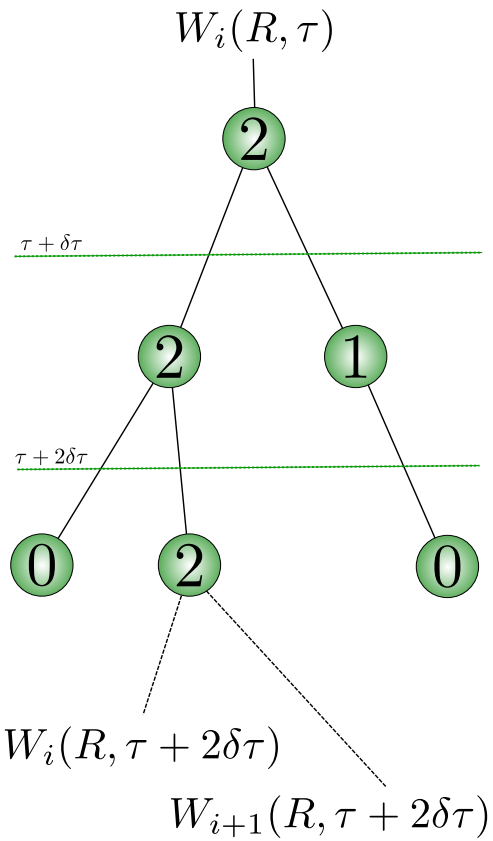

Figure: Branching illustrated. The integer values represent $\overline{G}_{\mathrm{B}}$.

Diffusion

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Anisotropic diffusion process. The quantum force pushes the walkers into regions of higher probability.

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

$$\mathbf{r}_{i+1} = \mathbf{r}_i + D\delta\tau\mathbf{F}(\mathbf{r}_i) + \xi, \tag{6}$$

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:

$$A(i \rightarrow j) = \min\{R_G(i \rightarrow j)R_\psi(i \rightarrow j)^2, 1\}, \tag{7}$$

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

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

and

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

End of section.

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